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Preliminary Experiments in a Research House to Investigate Contaminant Migration in Indoor Air

Geomet Technologies, Inc., Germantown, MD

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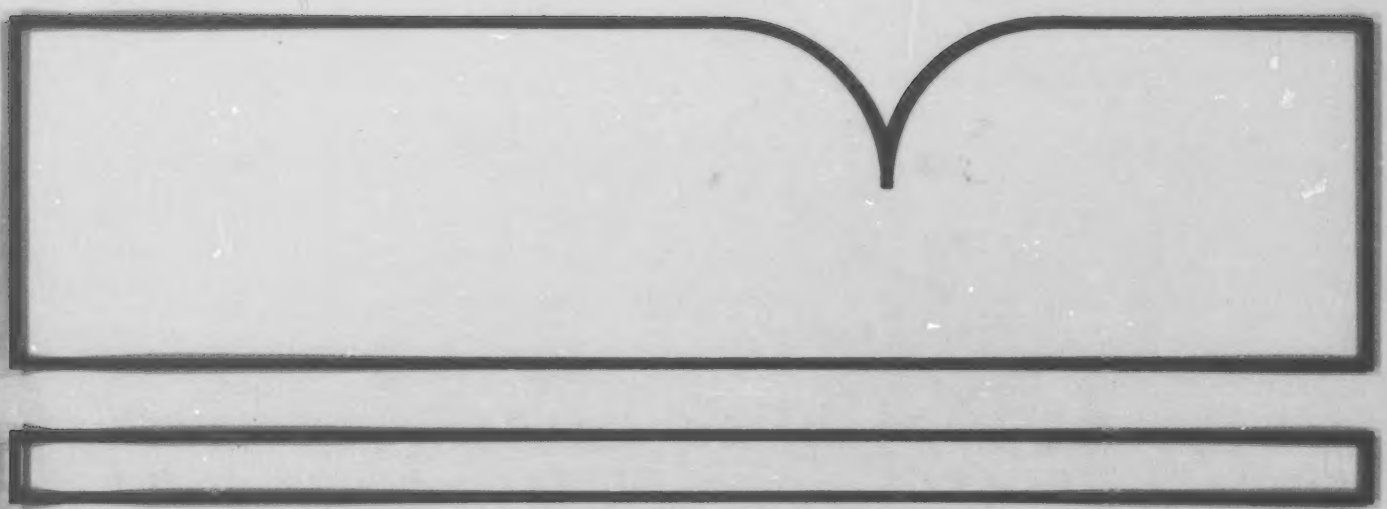

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16. Abstract (Limit: 200 words)

Controlled experiments were performed in an unoccupied research house to provide (1) a detailed characterization of the migration patterns of contaminants released indoors from consumer products and (2) a basis for assessment of the exposure implications of contaminant migration and the accuracy of currently used exposure assessment models. To enable relatively detailed spatial and temporal monitoring with readily available instrumentation, carbon monoxide (CO) was chosen as a surrogate contaminant for the investigation. A point source was simulated in the master bedroom by releasing CO from a pressurized tank through a pnematic line over a 1.25-hour period.

During the release period, measured CO concentrations typically were 3 to 4 times higher in the release area than in other areas on the floor of release. Within an hour after the release was terminated, concentrations approached spatial uniformity even though a central air circulation fan that would have promoted contaminant migration was turned off as part of the experimental design. A single-chamber indoor air quality model provided closer approximation of passive than active exposures. Use of a two-chamber model resulted in better estimates of each type of exposure.

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PRELIMINARY EXPERIMENTS IN A RESEARCH HOUSE TO INVESTIGATE CONTAMINANT MIGRATION IN INDOOR AIR

by

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EXECUTIVE SUMMARY

Over recent years, advances have been made in the development and application of methods for the assessment of exposure to chemical contaminants released from consumer products to the indoor environment. In spite of these advances, there still exist significant gaps in our understanding of the behavior of contaminants following their release and the implication of this behavior for human exposure. In particular, the extent of passive exposure (i.e., that arising from contaminant migration to indoor air spaces from the space where a contaminant is released) is poorly understood.

The OTS exposure-assessment process has recognized passive exposure as an issue of concern; however, appropriate information to provide quantitative treatment of this issue is not currently available. As a result, significant uncertainties exist with regard to the accuracy of indoor air exposure estimates. The objectives of the investigation described in this report were (1) to perform a detailed characterization of contaminant migration patterns in an unoccupied research house through a series of controlled experiments, (2) to assess the exposure implications of contaminant migration, and (3) to assess the accuracy of currently used exposure assessment models and explore model refinements that could lead to improved estimates of active and passive exposures.

To enable detailed spatial and temporal monitoring with readily available instrumentation, carbon monoxide (CO) was chosen as a surrogate contaminant for the investigation. CO was released from a point source in the master bedroom of the research house at a constant, known rate over a period of 1.25 hours. A network of nine portable continuous CO detectors was arrayed to measure horizontal and vertical concentration gradients in each of three configurations--(1) in the release area, (2) down a connecting hallway, and (3) in entrances to nearby bedrooms. An anchor string of three vertically arrayed detectors located just outside the entrance to the master bedroom provided continuity across the three different arrays of detectors. In addition, a stationary network of sampling locations representing likely passive exposure sites was sampled on a rotating basis with a nondispersive infrared analyzer. The simulated contaminant release was performed once in the morning and once in the afternoon for each array of CO detectors. Ancillary parameters such as outdoor CO concentrations, meteorological conditions, and air infiltration rates were also monitored.

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During the release period, measured CO concentrations typically were 3 to 4 times higher in the release area than in other upstairs areas of the house. However, within 45 to 60 minutes after the release was terminated, concentrations throughout the upstairs of the house approached spatial uniformity, even though a central air circulation fan that would have promoted contaminant migration was turned off as part of the experimental design. Some evidence of contaminant migration to the downstairs living area of the house was observed during selected experiments, but the downstairs concentrations were substantially lower that those upstairs. Variable vertical gradients in CO concentrations in the release area and along migration pathways suggested that a fairly complex system of forces is involved in the mixing and transport of contaminants.

Interestingly, a single-chamber model--similar to that currently used in OTS assessments of active exposures in residential environments--provided a closer approximation of passive than active exposures. Use of a two-chamber model resulted in better estimates of each type of exposure. Thus, even though a complex set of forces may underlie contaminant mixing and transport patterns, the concept of treating general interchamber airflow patterns as a steady-state condition into which consumer-product emissions are injected and transported appears valid and useful for improving exposure estimates.

To provide a basis for continued refinements and improvement to currently used models for exposure assessments, additional research house experiments need to be performed for a wider variety of release types and surrounding conditions. A detailed stationary monitoring network should be configured so that the experimental results can be easily compared. Future contaminant-migration experiments should include measurement of time-varying and integrated airflows as a routine component. In addition, the transferability of results from research houses to different housing types should be assessed by replicating selected experiments in a limited number of local residences.

To increase the applicability of exposure assessment models to a variety of housing types in different areas of the country, results of PFT measurements that are used to quantitate time-averaged airflow rates among selected zones of a residence should be analyzed as soon as these results are assembled in a computer-accessible format.

In parallel with expanded data collection, assimilation, and analysis efforts, activities to refine and improve current exposure assessment models should be initiated. This process should begin with the development of a generalized multichamber model and continue with refinements and expansions as critical inputs are obtained through supplemental efforts such as those recommended in this report.

PRELIMINARY EXPERIMENTS IN A RESEARCH HOUSE TO INVESTIGATE CONTAMINANT MIGRATION IN INDOOR AIR

1. INTRODUCTION

1.1. Background

Over recent years, advances have been made in the development and application of methods for the assessment of exposure to chemical contaminants released from consumer products to the indoor environment. An overall analytical structure has evolved to guide such evaluations, as have a variety of methods for calculating the indoor air contaminant concentrations to which receptors are exposed. Data bases quantifying consumer product use patterns and the chemical makeup of many consumer products have also been developed to support the application of the assessment process.

In spite of these steps, significant gaps exist in our understanding of contaminant behavior following release and the implication of this behavior for human exposure. In particular, the extent of passive exposure (i.e., that arising from contaminant migration to indoor air spaces from the space where a contaminant is released) is poorly understood.

The OTS exposure assessment process has recognized passive exposure as an issue of concern; however, appropriate information to provide quantitative treatment of this issue is currently lacking. As a result, significant uncertainties exist regarding the accuracy of indoor air exposure estimates. Thus, specific needs exist (1) to investigate the issue of passive exposure to determine whether it warrants further attention and (2) if so, to develop strategies for obtaining appropriate levels of quantitation.

In a recent report (GEOMET 1987a), average interior airflows and air infiltration rates measured with multiple perflourocarbon tracers (PFTs) for a typical residence were used as inputs to a multichamber indoor air quality model. This model was used to demonstrate the implications of passive exposure to chemical substances released from a consumer product within any of three zones in the house. For one of these cases, it was shown that within 2 hours after the 10-minute release period, concentrations were higher in another zone than in the zone where the substance was released. This analytical exercise demonstrated that the issue of passive exposures to chemical substances released from consumer products warrants concern and further investigation.

1.2. Objectives and Scope

The results of the analysis described above indicated that a data base maintained by Brookhaven National Laboratory, which contains results from PFT measurements in approximately 4,000 U.S. residences, may be a valuable input to future exposure assessments concerning the use of consumer products in residential environments. However, the PFT measurement technique is generally limited to quantifying average airflows over time periods of several days or longer. Consequently, the use of such data may still introduce inaccuracies in exposure assessments because many consumer products are used for shorter durations on the order of hours or minutes.

In concept, general airflow patterns derived from PFT measurements can be treated as a steady-state or slowly changing condition into which emissions from consumer products are injected and transported. Although this concept provides for facile incorporation of readily available data, it represents an untested extrapolation.

Consequently, a limited series of experiments was designed to quantify contaminant migration over detailed temporal and spatial scales in an unoccupied research house maintained by GEOMET. These experiments were exploratory in nature and were intended to improve our understanding of underlying physical processes rather than to mimic any specific exposure scenario. The major objectives of this effort were as follows:

- To examine the basic time scales and variations for contaminant migration to adjacent airspaces;
- To examine the relative levels and durations of passive exposure in adjacent airspaces due to contaminant migration;
- To examine the dilution effects of contaminant migration to adjacent rooms and air exchange with the outdoors; and
- To assess the ability of single- or multi-chamber models to predict active and passive exposures.

The experimental design involves the controlled release of a surrogate contaminant in one room of the research house and monitoring of contaminant mixing and migration to other rooms through a detailed network of sensors. The results of these

experiments will enable a quantitative assessment of the utility of existing and readily obtainable data relating to interroom airflows.

The research setting, experimental design, and measurement methods are described in Section 2 of this report. Experimental results are presented in Section 3 and modeled in Section 4. The implications of the results are discussed in Section 5 in terms of model accuracies, applicability of existing data on interior airflows, and future research needs. Conclusions and recommendations stemming from this investigation are outlined in Section 6.

2. EXPERIMENTAL DESIGN AND RESEARCH METHODS

This section describes the setting in which experiments were conducted, together with contaminant release and monitoring methods. Measurement techniques for ancillary parameters such as outdoor meteorological conditions, indoor temperatures, and air infiltration rates are also described. The section concludes with a description of quality assurance/control, data processing, and analysis procedures. Portions of this section are extracted from a recent GEOMET report (1987b) describing sampling and analytical protocols for the investigation.

2.1. Research Setting

GEOMET's research house facility consists of two bilevel, wood-frame houses that were constructed in the fall of 1982. The houses, located on adjacent lots in Gaithersburg, Maryland, are identically oriented, facing 19° east of north (i.e., north-northeast). Floor plans for the houses are shown in Figure 1. The main living area is upstairs; the downstairs area is divided into an unfinished living area and an integral garage. The total upstairs living area of each house is 130 m^2 (1400 ft^2). The upper and lower levels are connected by a stairway with one landing at the house entryway.

The research houses were constructed using "closed-wall" techniques. Siding, sheathing, insulation, vapor barrier, and windows were assembled at the factory to form complete wall panels. The completed wall panels were installed at the building site to form the building shell. Insulation for the research houses features a continuous polyethylene vapor barrier with glass fiber batts between the wall joints (R-value of 11). The attic contains 8 inches of loose fill insulation between the ceiling joists (R-value of 30).

Abbreviations that are used later in this report for selected rooms or areas of the house are also indicated in Figure 1.

2.2. Contaminant Release and Monitoring

The experimental strategy was designed to monitor contaminant history from a constant point source through three possible stages (Figure 2):

- Source cloud--in the immediate vicinity of the source, concentrations are controlled by the

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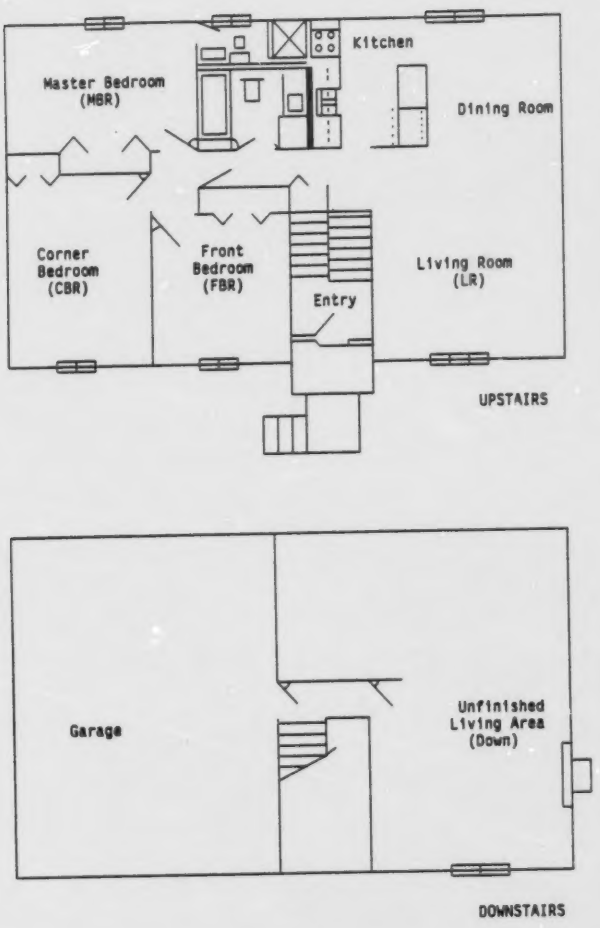


Figure 1. Floor plan of GEOMET research houses.

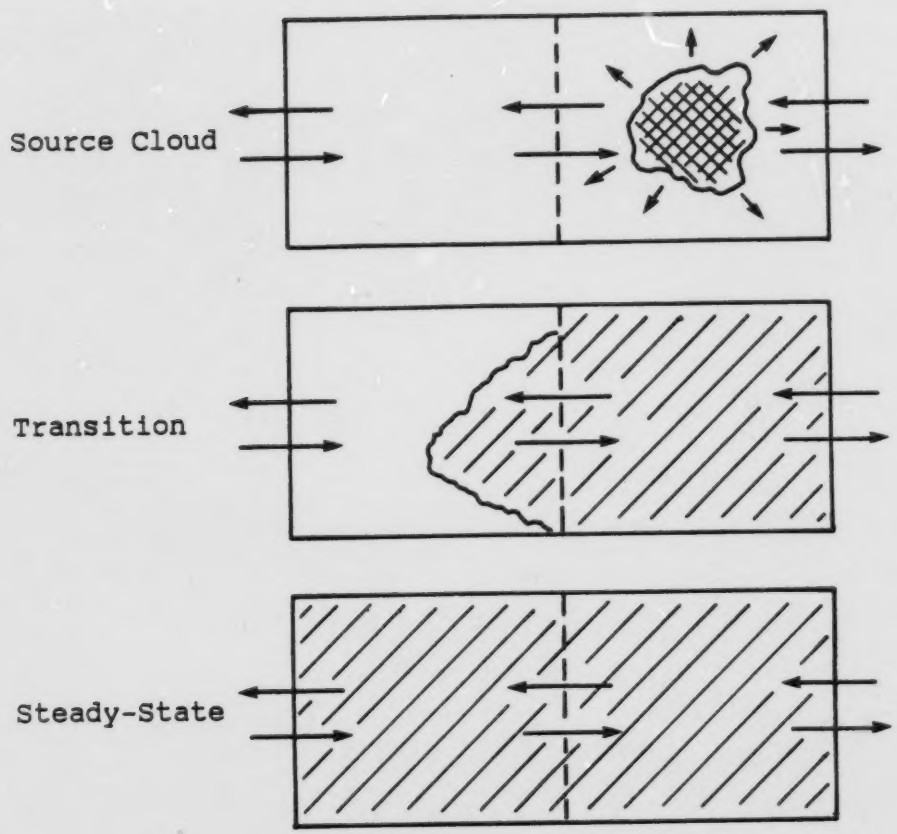


Figure 2. Three possible stages of contaminant history.

amount of material released and the dimensions of the source cloud;

- Transition--once the source cloud approaches the dimensions of the room, concentrations begin to be affected by air exchange and migration to adjacent airspaces; and

- Steady state--concentrations throughout the general airspace change in response to air exchange, room-to-room flows, and (as applicable) continuing emissions and chemical decay.

The basic experimental sequence began with a controlled release of a surrogate contaminant from the center of the master bedroom in one of the research houses. The measurement strategy involved a set of portable continuous analyzers that were arranged to form a sampling plane that was "walked" through the concentration patterns created by controlled repetition of a single-release scenario. General characteristics of the release scenario are summarized in Table 1.

Carbon monoxide (CO) was selected as the surrogate contaminant. CO was released from a pressurized tank located outdoors that contained approximately 1 percent CO in air. Pneumatic lines were used to direct the contaminant from the tank to the release point in the master bedroom; the gas feed was controlled externally so that the technician would not need to enter the house during the conduct of any experiment. To prevent undue mixing from momentum of the release flow, a ceramic frit was installed on the outlet at the release point. Based on a preliminary experiment, a release rate of 1.2 L/min and duration of 1.25 hours were chosen; these conditions resulted in short-term CO peaks on the order of 10 parts per million (ppm) in the master bedroom and concentrations below 5 ppm elsewhere in the house.

Evolution of the source-cloud and transition stages was monitored by arranging nine portable continuous CO monitors (General Electric Model 15ECS3C03) to form a vertical sampling plane. The vertical sampling plane was made up of three vertical sampling strings. As illustrated in Figure 3, the nominal floor-to-ceiling dimension of the upstairs of the research house is 2.3 meters. Sampling heights of 0.38, 1.16, and 1.93 meters were specified for each vertical string to systematically divide the vertical sampling plane into three layers that were each 0.77 meters deep.

Table 1. Characteristics of Release Scenario

1. General conditions

   - All exterior openings (doors, windows) closed
   - All interior doorways on main floor open
   - Doorway to downstairs opened
   - Doorway to garage closed
   - Operation of central circulation fan suppressed

2. Release conditions

   - Location--geometric center of master bedroom
   - Rate--1.2 L/min from tank containing 0.9844 percent CO in air
   - Duration--1.25 hours

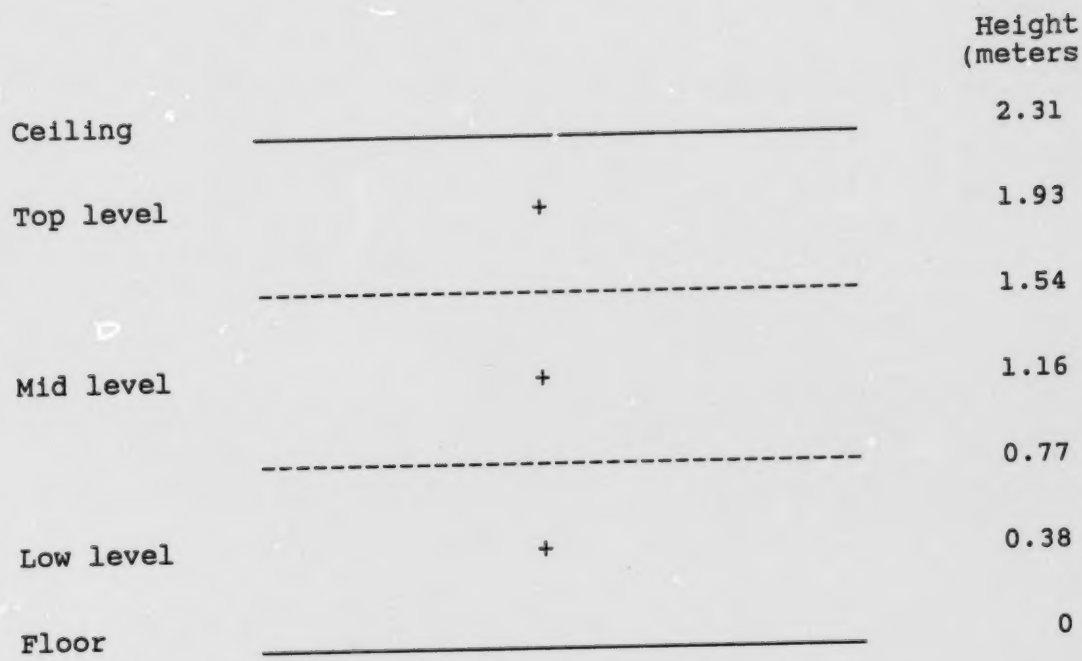


Figure 3. Spacing of portable continuous monitors to form a vertical sampling string. Crosses (+) denote monitoring height for top, mid, and low levels situated between floor and ceiling.

To provide continuity from experiment to experiment, one location was designated as the anchor point for all arrangements of the vertical sampling strings. This point (designated as point A in Figure 4) was centrally located in the hallway equidistant from the doorways of all three bedrooms. For the initial experiment, vertical strings 2 and 3 were set up to bracket the release point, giving a sampling plane defined by the anchor plus positions S_2 and S_3 indicated in Figure 4.

For experiment type 2, vertical strings 2 and 3 were relocated to the hallway (positions H_2 and H_3 in Figure 4). For experiment type 3, the sampling plane was folded to extend into the corner bedroom and the front bedroom by placing sampling strings 2 and 3 at locations D_2 and D_3, respectively.

Data from the nine portable monitors were collected every 6 seconds and processed by a data logger for storage as 1-minute averages during each experiment.

A stationary sampling network was operated to continually measure CO concentrations in each major room of the research house, except for the room of release. This second network, also indicated in Figure 4, consisted of a single continuous analyzer (Beckman Model 886) that was automatically sequenced among five sampling points on a 3-minute schedule, providing a measurement of each point every 15 minutes. For consistency with previous monitoring protocols, indoor CO measurements with the stationary network were taken at a height of 1.07 meters.

Experiments were conducted during the period December 1-4, 1987. As summarized in Table 2, the controlled-release scenario was conducted twice for each array of the vertical strings--once during morning hours (10:00 to 11:15 a.m.) and once during evening hours (4:00 to 5:15 p.m.). The afternoon experiment for type 2 was repeated, and the data from this seventh experiment were held in reserve. To restore indoor CO concentrations to background levels between morning and evening experiments, windows were opened at 2:00 p.m. and closed at 3:00 p.m., allowing an hour for cessation of any air movement patterns due to the window openings.

A possible source of interference for these experiments was local automobile traffic. However, historical data from the research site indicated that brief outdoor transients coinciding with early morning and late afternoon traffic peaks would be relatively rare and on the order of 5 ppm or lower should they occur. The extent of interference from any outdoor CO spikes was quantified with the stationary monitoring network, through which outdoor CO concentrations were measured every 15 minutes.

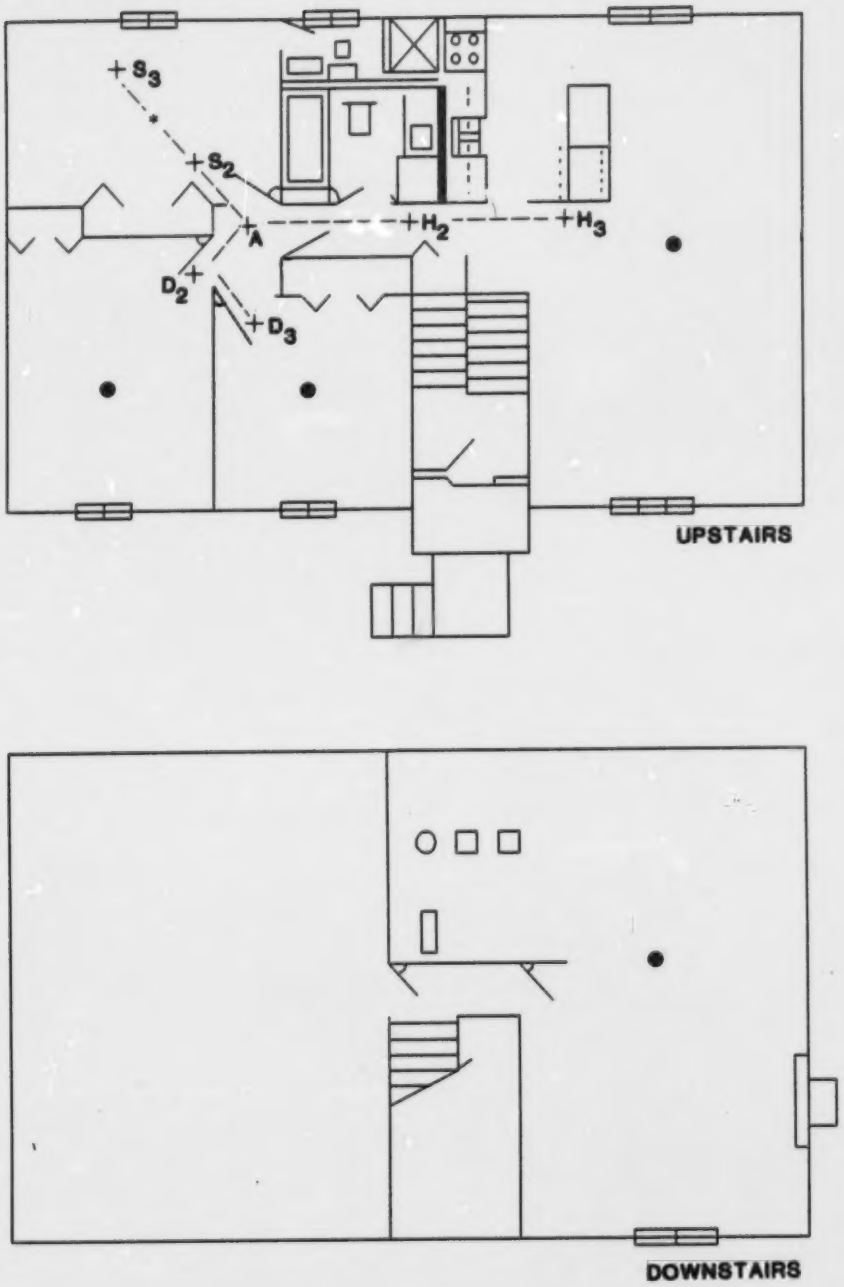


Figure 4. General locations of the release point (denoted by an asterisk), the vertical sampling planes (denoted by crosses joined by broken lines), and the stationary monitoring network (denoted by filled circles).

Table 2. Sequence of Contaminant-Release Experiments

Date	Release period	Experiment type (array of vertical sampling strings)
December 1	4:00 to 5:15 p.m.	Type 1
December 2	10:00 to 11:15 a.m.	Type 2
	4:00 to 5:15 p.m.	Type 2
December 3	10:00 to 11:15 a.m.	Type 3
	4:00 to 5:15 p.m.	Type 3
December 4	10:00 to 11:15 a.m.	Type 1
	4:00 to 5:15 p.m.	Type 2

2.3. Ancillary Measurements

The GEOMET research house facility contains a complete indoor and outdoor network of continuous sensors for indoor environmental conditions, operating status of major appliances, and meteorological conditions outdoors. The parameters selected to assist in data interpretation included indoor air temperature and the meteorological parameters of windspeed and direction, solar radiation, outdoor air temperature, and precipitation. Siting criteria for these parameters are listed in Table 3.

In addition to environmental parameters, air infiltration rates were measured using the tracer-dilution method (ASTM 1981), with sulfur hexafluoride (SF_6) as the tracer. Before each experiment, SF_6 was injected into the research house with an automated system that provided rapid mixing through the central forced-air heating and cooling system. Following the period of SF_6 injection, the air circulation system was kept off throughout each experiment. Indoor sampling locations for SF_6 were identical to those used for the stationary CO monitoring network; a single analyzer was used to sequentially sample each location, enabling calculation of air infiltration rates over periods as short as 15 minutes. The instruments used to monitor SF_6 concentrations and environmental parameters are listed in Table 4.

2.4. Quality Assurance and Control Procedures

Data quality objectives were stipulated in the protocol document (GEOMET 1987b) in terms of accuracy, precision, and completeness of data collected during the experiments. For most parameters, the targeted accuracy and precision levels were ±10 percent; the targeted completeness of the data across all measurement parameters and experiments was 95 percent. Specific procedures used to ensure the collection of high-quality data included external audits, multipoint calibrations, zero and span checks, and additional routine activities performed by technicians responsible for conducting the experiments and maintaining the research houses.

The most recent external audit at the research houses, conducted during September 1987, involved (1) challenging GEOMET's gas analyzers with known concentrations of National Bureau of Standards (NBS)-traceable standard gases and (2) colocating NBS-traceable instruments with GEOMET's meteorological and indoor-environment sensors for parallel monitoring and comparison of instrument responses. Audit parameters of relevance to this investigation included the Beckman analyzer used for the stationary CO network, four of the nine portable GE CO detectors, the SF_6 analyzer, all outdoor meteorological sensors, and a subset of the indoor-temperature sensors.

Table 3. Specifications for Ancillary Measurement Parameters

Parameter	Number of indoor sites	Number of outdoor sites	Location
Windspeed	0	1	10 m above ground[a]
Wind direction	0	1	10 m above ground[a]
Solar radiation (total)	0	1	Roof of house[a]
Air temperature	8	1	Indoor: Centroid of each major room[b]; Outdoor: 1.5 m above ground[a]
Precipitation	0	1	Gauge opening 0.3 m above ground[a]
Air exchange rate	4	0	Colocated with stationary probes for CO

[a] In general accordance with Section 3.0 of the EPA Quality Assurance Handbook for Air Pollution Measurement Systems: Volume IV. Meteorological Measurements (EPA-600/4-82-060).

[b] In accordance with criteria established through previous experimentation reported in "Energy Use, Infiltration, and Indoor Air Quality in Tight, Well-Insulated Residences" (EPRI Report No. EA/EM-4117), prepared by GEOMET for the Electric Power Research Institute.

Table 4. Instrumentation for Ancillary Measurement Parameters

Parameter	Instrumentation	Manufacturer	Model
SF_6	Gas chromato-graph/electron capture detector	S-Cubed	215BGC
Temperature	Thermistor	Omega	0L-700
Windspeed	Anemometer	Climatronics	WM-III
Wind direction	Vane	Climatronics	WM-III
Solar radiation	Pyranometer	Matrix	MKI-G
Precipitation	Tipping bucket	Qualimetrics	6021A

Multipoint calibrations were conducted for all gas analyzers at the beginning and end of the 4-day period during which contaminant-release experiments were conducted. In addition, zero and span checks were performed before each morning experiment was conducted, the results of which were recorded on control charts. Based on historical performance data, control limits of ±0.75 ppm at zero and ±1.5 ppm at span (9 ppm) were established for all CO monitors. Any CO monitor exhibiting a response outside the control limits was recalibrated before a new experiment was initiated.

On arrival at the research houses each day, the technician first performed routine operational checks of various types of equipment. Findings and observations were recorded on a daily checklist form (Figure 5) to establish the degree of general readiness for planned activities. The experiments were designed to operate without intervention by the technician. Principal areas of attention included physically rearranging the detailed network of CO analyzers, verifying the readiness of the analyzers (based on zero and span checks) and data acquisition systems, and initiating/terminating the source release. Measurements of air infiltration and other auxiliary parameters proceeded through a computer-controlled system with specified intervals for sampling and recording instrument signals.

Critical daily actions were recorded on an operational checklist (Figure 6). A typical daily schedule involved the following sequence of events:

(1) After making the types of operational checks described above, the data file containing results from the previous day's experiments was closed and a new file was opened for recording results from the current day's experiments.

(2) After verifying that concentrations from the previous afternoon's experiment had receded to acceptable levels, the technician reconfigured the detailed network of CO analyzers as necessary and performed zero and span checks.

(3) Source-feed connections to the release room were checked and the morning release was initiated. The technician reviewed the progress of the experiment by monitoring selected parameters on the CRT screen for the central data acquisition system.

HVAC on-line: 14 15

Gas [ ] [ ]
Electric [ ] [ ]
Other [ ] [ ]

Date: _____
J.D.: _____
Time: _____
Technician: _____

Daily Checklist - Instrumentation

A. Performance Checks (Verify reasonableness of data and check)

14	15	Channels	Parameters
[ ]	[ ]	A0 — C07	Room temperature
[ ]	[ ]	C10 — C15	Energy
[ ]	[ ]	D0 — E03	HVAC and duct temperatures
[ ]	[ ]	E04 — E09	RH and room velocity
[ ]	[ ]	E10 — F06	Pressure and velocity
[ ]	[ ]	G04 or G01	Furnace fan status change
[ ]	[ ]	H03	Furnace gas counter (verify operation)
[ ]	[ ]	I0 — I15	Pollutants & meteorology

Record screen display values for the following (during HVAC operation):

14	15		14	15	
___	___	A0 (MBR Temp)	___	___	D11 (Supply Temp)
___	___	B4 (LR Temp)	___	___	D14 (Return Temp)

B. Status/Logical Checks (Verify status or parameter change after system begins operation)

14	15	
[ ]	[ ]	Furnace fan
[ ]	[ ]	Furnace gas valve
[ ]	[ ]	Supply temperatures increase
[ ]	[ ]	Furnace thermocouple
[ ]	[ ]	HVAC system initiated at appropriate room temperature

C. Instrumentation checks (verify operation, flows, reasonableness of data--insert "1" if operational or "0" if off-line)

		1	2	3	4	5	
[ ]	SF_6 zone sequence	[ ]	[ ]	[ ]	[ ]	[ ]	RADON
[ ]	Pollutant zone sequence	[ ]	[ ]	[ ]	[ ]	[ ]	RADON PROGENY
[ ]	DAS clocks	[ ]	Pressure sensors (specify any off-line) _____				
[ ]	SF_6 Analyzer	[ ]	Halocarbons				
	Pollutant Analyzers						
[ ]	NO_x/NO A	[ ]	CO-A				
[ ]	NO_x/NO B	[ ]	CO-B				
[ ]	CO_2-A	[ ]	O_2				
[ ]	CO_2-B	[ ]	Other: _____				

D. Comments: _____

Figure 5. Daily checklist form.

CHECKLIST--CONTAMINANT MIGRATION EXPERIMENTS

A. Experimental Configuration: _____

B. Instrumentation

GE CO Detectors

Channel	Serial No.	Status
1	_____	[ ]
2	_____	[ ]
3	_____	[ ]
4	_____	[ ]
5	_____	[ ]
6	_____	[ ]
7	_____	[ ]
8	_____	[ ]
9	_____	[ ]

Placement in Sampling Plane

7	4	1
8	5	2
9	6	3

C. Source Release Data

Daytime

Start Time: _____ Stop Time: _____

Flow: _____

Tank Concentration

_____ % CO in Air

Overnight

Start Time: _____ Stop Time: _____

Flow: _____

Tank Concentration

_____ % CO in Air

D. Data Files

Campbell Datalogger

File Name: _____
Start: _____
End: _____

Clock Status [ ]

Site DAS

File Name: _____
Start: _____
End: _____

Clock Status [ ]

Comments: _____
_____
_____
_____

Figure 6. Operational checklist for experiments.

(4) After completion of the morning experiment, the technician verified that concentrations had declined to acceptable levels and initiated the afternoon release of CO. The afternoon experiment then proceeded to automatic shutdown of the CO release and continuing measurements under program control.

2.5. Data Processing and Analysis Procedures

All instrument signals were scanned, averaged, and recorded at prescribed intervals by computer-controlled data acquisition systems. Instruments measuring meteorological parameters were scanned at 1-minute intervals and recorded as hourly averages. Measurements with the stationary sampling network for CO and SF_6 were recorded at 3-minute intervals corresponding to the times at which various locations were sequentially sampled. A separate data acquisition system was devoted to the network of nine CO detectors to enable the recording of 1-minute averages at each sampling site. All instrument outputs were recorded as voltages on IBM-PC-compatible diskettes.

Calibration factors (slope and intercept) derived from multipoint calibrations were applied to the raw data at GEOMET's data center through programs implemented on IBM personal computers and compatibles. The calibrated data were reviewed for unreasonable values such as negative concentrations and sharp excursions from smooth trends (e.g., a temporary decline of one data point to near-zero values during a period of otherwise steady growth). Questionable values were flagged to alert analysts to sections of valid and invalid data.

Data analysis efforts were keyed to the basic objective of these experiments--exploring the implications of contaminant migration patterns for current methods of estimating human exposures. Fundamental avenues of analysis included (1) comparisons across experiments through graphical and statistical methods, (2) comparisons of measured values with those predicted by currently used models, and (3) evaluations of model refinements.

Initial stages of data analysis focused on basic concentration profiles as well as similarities and differences across different experiments. This comparative analysis was applied to CO concentrations as well as to air infiltration rates, indoor temperatures, and meteorological conditions. In particular, the spatial and temporal profiles of CO concentrations near the doorway to the master bedroom were assessed for consistency across experiments; the vertical string of CO analyzers at this

location was the anchor point for linking results across the three types of experiments.

The functional relationships among the vertical strings constituting the detailed CO sampling network and stationary CO monitoring sites are illustrated in Figure 7. To summarize and integrate results across experiments, statistics such as peak and average CO concentrations were used in addition to graphical summaries.

The general mass balance model currently used for indoor air exposure assessments was applied to estimate indoor concentrations in the region of the source and at remote locations, based on measured values of air infiltration rates, source release rates, and outdoor CO concentrations. The general framework for mass balance models is summarized in Appendix A.

Model residuals (algebraic differences between calculated and measured concentrations) were analyzed to identify model assumptions or outdoor conditions that led to significant differences as well as good correspondence. Particular attention was given to identifying conditions where the single-chamber model provided poor estimates of passive or active exposures.

The final stages of data analysis explored various avenues of model refinement including multichamber models for estimating passive exposures. Results from previous PFT measurements at the research house under similar outdoor conditions were included as inputs to the multichamber model.

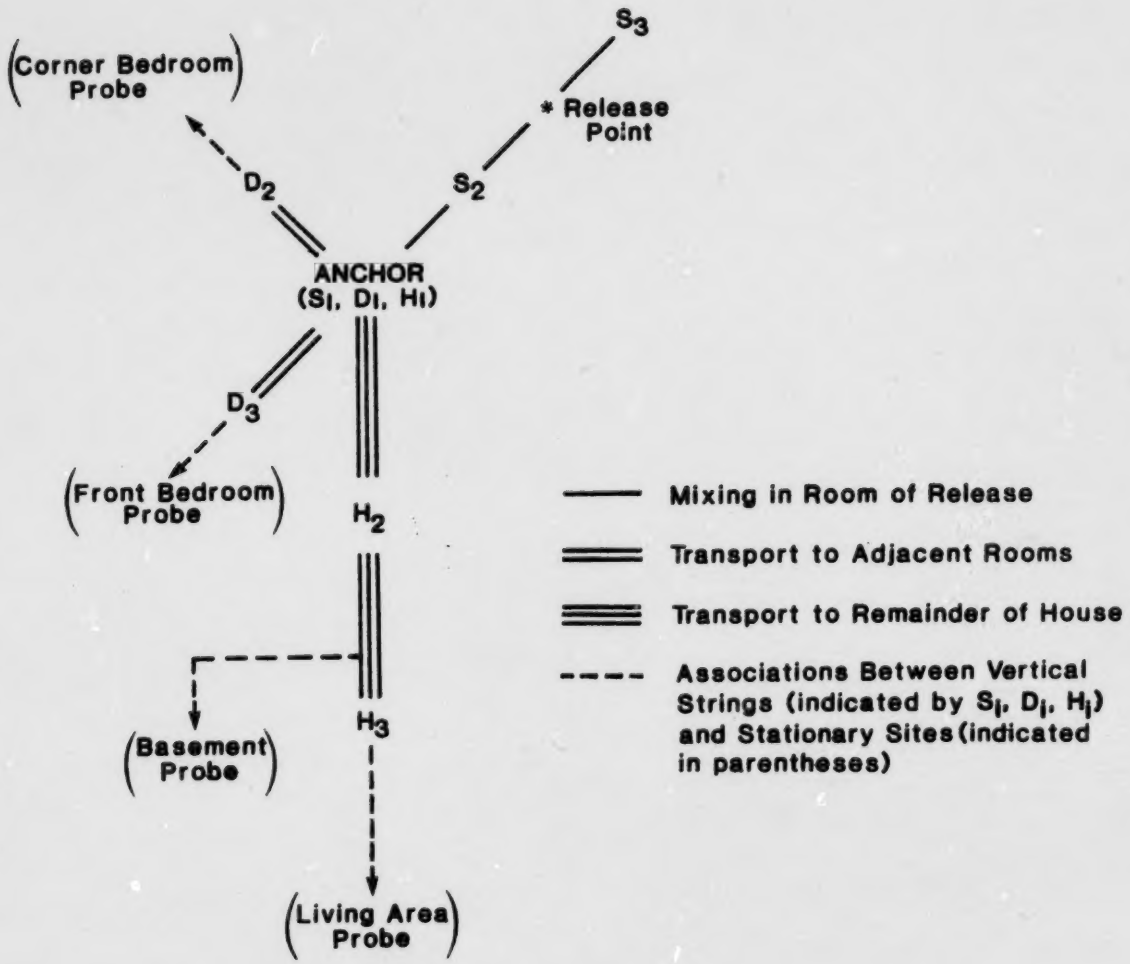


Figure 7. Functional relationships among vertical sampling strings of the detailed monitoring network and stationary monitoring sites.

3. ANALYSIS OF EXPERIMENTAL RESULTS

Outdoor conditions prevailing during each of the experiments are summarized in Section 3.1, and data quality levels associated with critical measurement parameters are summarized in Section 3.2. Concentration profiles for each experiment are presented in Section 3.3, and the results across all experiments are integrated in Section 3.4.

3.1. Experimental Conditions

Sampling was conducted during the first 4 days of December 1987. Three different configurations of portable CO detectors were used in the master bedroom, hallway, and other bedrooms. Two experiments were performed for each configuration, one starting at 10 a.m. and another starting at 4 p.m.

Both ambient and indoor conditions can influence the concentrations and rates of migration of contaminants in indoor environments. Indoor temperatures, ambient carbon monoxide concentration, air infiltration rate, and meteorological conditions (winds, temperature, and solar radiation) were used as a basis for summarizing the prevailing conditions during each experiment. Average values, standard deviations, and ranges for these parameters during the 4-hour period of CO release and decay for each experiment are given in Table 5.

During each of the six experiments, both indoor and outdoor temperatures remained within 10 percent of the mean value. Although temperature differences between the morning and afternoon experiments were observed, the overall temperature difference between indoors and outdoors was quite similar across the pair of experiments for each configuration of CO detectors. Air infiltration rates usually were slightly higher during the afternoon than morning experiments.

The average windspeed was typically as high or higher during morning than afternoon experiments. Solar radiation levels were also higher during morning than afternoon experiments, mainly because the afternoon decay period included hours after sunset. The highest ambient CO concentration during any experiment was 1.4 ppm. This relatively low level, coupled with upstairs air infiltration rates averaging about 0.3 air changes per hour, implies that outdoor CO concentrations had negligible impacts on indoor concentration levels.

Table 5. Summary of Prevailing Conditions During Each Experiment

Date/period of experiment	Parameter	Average	Standard deviation	Range
Part A: Experiment Type 1--Vertical Sampling Strings in Master Bedroom				
Morning (12/04/87)	Air temperature (°F)			
	Ambient outdoor	38.2	0.7	37.6 to 39.1
	Master bedroom	63.3	1.3	61.9 to 64.9
	Corner bedroom	63.0	1.2	61.7 to 64.6
	Front bedroom	63.5	1.3	62.1 to 65.1
	Hallway	64.5	1.3	63.2 to 66.2
	Living room	64.2	1.3	62.8 to 65.8
	Downstairs	63.0	0.9	62.0 to 64.1
	Upstairs infiltration rate (h^{-1})	0.30	0.02	0.28 to 0.33
	Ambient outdoor CO (ppm)	0.8	0.1	0.6 to 0.9
	Windspeed (mi/h)	5.0	0.6	4.4 to 5.8
	Wind direction (degrees)	291	11.5	278 to 303
	Solar radiation (Btu/ft^2)	21	5.4	14 to 16
Afternoon (12/01/87)	Air temperature (°F)			
	Ambient outdoor	44.3	0.6	43.9 to 45.2
	Master bedroom	64.6	1.3	63.3 to 66.2
	Corner bedroom	64.4	1.3	63.0 to 66.1
	Front bedroom	64.7	1.3	63.3 to 66.3
	Hallway	65.6	1.1	64.4 to 67.0
	Living room	65.3	1.2	64.0 to 66.8
	Downstairs	64.1	0.7	63.3 to 65.0
	Upstairs infiltration rate (h^{-1})	0.29	0.07	0.23 to 0.36
	Ambient outdoor CO (ppm)	0.7	0.5	0.3 to 1.4
	Windspeed (mi/h)	2.8	1.1	1.8 to 4.3
	Wind direction (degrees)	231	22.1	211 to 258
	Solar radiation (Btu/ft^2)	1	2	0 to 4

(Continued)

Table 5. Summary of Prevailing Conditions During Each Experiment (Continued)

Date/period of experiment	Parameter	Average	Standard deviation	Range
Part B: Experiment Type 2--Vertical Sampling Strings In Hallway				
Morning (12/02/87)	Air temperature (°F)			
	Ambient outdoor	41.7	1.2	40.0 to 42.7
	Master bedroom	67.9	1.0	66.9 to 69.2
	Corner bedroom	66.3	0.4	66.1 to 67.0
	Front bedroom	66.6	0.4	66.4 to 67.2
	Hallway	68.3	0.4	67.8 to 68.7
	Living room	68.0	0.6	67.2 to 68.7
	Downstairs			
	Upstairs infiltration rate (h^{-1})	0.30	0.02	0.26 to 0.32
	Ambient outdoor CO (ppm)	0.3	0.2	0.0 to 0.4
	Windspeed (mi/h)	10.2	2.1	7.7 to 12.2
	Wind direction (degrees)	310	52.2	263 to 357
	Solar radiation (Btu/ft^2)	95	35.8	42 to 121
Afternoon (12/02/87)	Air temperature (°F)			
	Ambient outdoor	36.6	2.0	34.6 to 39.2
	Master bedroom	63.6	2.2	61.2 to 66.3
	Corner bedroom	62.6	1.8	60.6 to 64.7
	Front bedroom	63.0	1.8	61.1 to 65.2
	Hallway	64.9	1.7	63.0 to 66.9
	Living room	63.8	1.8	61.8 to 66.0
	Downstairs	62.3	0.9	61.3 to 63.4
	Upstairs infiltration rate (h^{-1})	0.36	0.06	0.29 to 0.42
	Ambient outdoor CO (ppm)	0.7	0.2	0.5 to 1.0
	Windspeed (mi/h)	6.6	1.4	5.1 to 8.2
	Wind direction (degrees)	333	3.5	329 to 337
	Solar radiation (Btu/ft^2)	2.5	5	0 to 10

(Continued)

Table 5. Summary of Prevailing Conditions During Each Experiment (Concluded)

Date/period of experiment	Parameter	Average	Standard deviation	Range
Part C: Experiment Type 3--Vertical Sampling Strings in Doorways of Adjacent Bedrooms				
Morning (12/03/87)	Air temperature (°F)			
	Ambient outdoor	41.0	0.8	40.0 to 41.7
	Master bedroom	66.2	0.8	65.1 to 66.9
	Corner bedroom	65.1	0.5	64.5 to 65.6
	Front bedroom	65.5	0.6	64.8 to 66.1
	Hallway	66.6	0.6	65.8 to 67.1
	Living room	66.9	0.6	66.0 to 67.4
	Downstairs			
	Upstairs infiltration rate (h^{-1})	0.26	0.04	0.22 to 0.32
	Ambient outdoor CO (ppm)	0.2	0.3	0.0 to 0.5
	Windspeed (mi/h)	6.4	0.4	5.9 to 6.8
	Wind direction (degrees)	194	7.1	189 to 205
	Solar radiation (Btu/ft^2)	95	31.3	51 to 123
Afternoon (12/03/87)	Air temperature (°F)			
	Ambient outdoor	40.3	1.8	37.9 to 42.0
	Master bedroom	61.9	1.4	60.4 to 63.6
	Corner bedroom	62.0	1.5	60.4 to 63.8
	Front bedroom	62.2	1.3	60.8 to 63.9
	Hallway	63.4	1.2	62.0 to 64.9
	Living room	63.0	1.3	61.6 to 64.7
	Downstairs	62.5	1.0	61.5 to 63.7
	Upstairs infiltration rate (h^{-1})	0.31	0.03	0.28 to 0.35
	Ambient outdoor CO (ppm)	0.3	0.2	0.1 to 0.5
	Windspeed (mi/h)	6.6	1.2	5.2 to 8.2
	Wind direction (degrees)	175	54.1	97 to 214
	Solar radiation (Btu/ft^2)	1.5	1.7	0 to 4

3.2. Data Quality

Data quality levels associated with this investigation are summarized in this subsection in terms of measurement accuracy and precision. The focus is on the primary measurement parameter for the investigation--concentrations of the surrogate contaminant (CO). Results from a recent external performance audit, as well as multipoint calibrations and zero and span checks covering the specific period of investigation, were used as inputs to the assessment of data quality for this parameter. The performance of measurement systems for air infiltration rates and meteorological parameters is also characterized.

During September 1987, an external performance audit was conducted at GEOMET's research house facility by the Center for Environmental Quality Assurance of Research Triangle Institute (RTI 1987). Four of the CO detectors and the Beckman CO analyzer used in this project were included in the audit. Each analyzer was challenged with zero air and with CO concentrations of 5, 10, 20, 30, and 45 ppm. The audit results are summarized in Table 6 in terms of a regression equation expressing the relationship between analyzer response and audit concentration. Perfect agreement would be indicated by a slope of one, an intercept of zero, and a correlation coefficient of one. As shown in the table, slopes for all analyzers were within ±0.01 of unity, and intercepts were relatively small in magnitude for all analyzers except GE detector #108, which exhibited a negative bias of 1 ppm. All correlation coefficients were either 1 or 0.9999.

The accuracy and precision of the analyzers at an audit concentration of 10.34 ppm are summarized in Table 7. The accuracy objective of 10 percent was met or exceeded by all detectors. Aside from GE detector #108, which had an accuracy level of -10 percent due to the 1-ppm negative bias, the accuracy of the detectors was within 3 percent. The precision across detectors was ±5 percent, well within the objective of ±10 percent. Thus, these results indicate that the performance of the CO analyzers was quite satisfactory at the time of the audit.

Accuracy and precision of all nine CO detectors and the Beckman analyzer used during the investigation are shown in Table 8, based on responses to a final calibration concentration of 9.06 ppm. The accuracy of the analyzers ranged from -2.4 to +2.5 percent, and the precision across all analyzers was ±1.4 percent. Thus, accuracy and precision levels at the final calibration were well within data quality objectives of ±10 percent.

Table 6. Summary of External Audit[a] Results for Five CO Analyzers

Analyzer	Regression of analyzer response on audit concentration		
	Slope	Intercept	Correlation coefficient
GE detector #142	0.99	-0.12	1.0000
GE detector #119	0.99	-0.07	0.9999
GE detector #108	1.01	-1.01	0.9999
GE detector #104	0.99	0.16	1.0000
Beckman model 866	1.00	0.26	1.0000

[a] Audit conducted on September 21, 1987.

Table 7. Accuracy and Precision of Five CO Analyzers at Audit Concentration of 10.34 ppm

Analyzer	Response, ppm	Accuracy, percent
GE detector #142	10.10	-2.3
GE detector #119	10.24	-1.0
GE detector #108	9.31	-10.0
GE detector #104	10.37	+0.3
Beckman model 866	10.79	+3.1
Average, all analyzers	10.16	
Standard deviation	0.54	
Precision, percent	±5.3	

Table 6. Summary of External Audit[a] Results for Five CO Analyzers

Analyzer	Regression of analyzer response on audit concentration		
	Slope	Intercept	Correlation coefficient
GE detector #142	0.99	-0.12	1.0000
GE detector #119	0.99	-0.07	0.9999
GE detector #108	1.01	-1.01	0.9999
GE detector #104	0.99	0.16	1.0000
Beckman model 866	1.00	0.26	1.0000

[a] Audit conducted on September 21, 1987.

Table 7. Accuracy and Precision of Five CO Analyzers at Audit Concentration of 10.34 ppm

Analyzer	Response, ppm	Accuracy, percent
GE detector #142	10.10	-2.3
GE detector #119	10.24	-1.0
GE detector #108	9.31	-10.0
GE detector #104	10.37	+0.3
Beckman model 866	10.79	+3.1
Average, all analyzers	10.16	
Standard deviation	0.54	
Precision, percent	±5.3	

Table 8. Accuracy and Precision of all CO Analyzers Used in the Investigation at Final Calibration[a] Input of 9.06 ppm

Analyzer	Response, ppm	Accuracy, percent
GE detector #037	9.12	+0.7
GE detector #104	9.07	+0.1
GE detector #108	8.84	-2.4
GE detector #119	9.11	+0.6
GE detector #123	8.87	-2.1
GE detector #130	9.00	-0.7
GE detector #142	9.07	+0.1
GE detector #147	9.29	+2.5
GE detector #153	9.11	+0.6
Beckman model 866	9.11	+0.6
Average, all analyzers	9.06	
Standard deviation	0.13	
Precision, percent	±1.4	

[a] Final calibration conducted on December 7, 1987.

Changes in slopes and intercepts for the CO detectors between beginning and ending calibrations are summarized in Table 9. Changes in slopes were minimal--7 percent at most and 2 percent or less for six of the nine detectors. Drift in the intercepts was somewhat more pronounced; eight of the nine detectors exhibited a downward drift in the intercept, averaging 0.5 ppm. This downward drift was most likely due to the sensitivity of the CO detector to temperature; as indicated in Section 3.1, indoor temperatures during the experiments were between 60 and 70°F because the central heating system was turned off during the conduct of each experiment.

Intermediate zero and span checks were performed on 36 occasions (nine detectors on 4 days each); in seven of these cases, detectors drifted to an out-of-control state. However, four of these cases were associated with a single detector (#108). In contrast to the beginning and ending calibrations that were performed in the laboratory adjacent to the house, zero and span checks were performed inside the research house so that the detectors would not be removed from the testing environment. Bags filled with zero and span gases were used for the zero and span checks, as opposed to multipoint calibrations that fed the gases directly to the detectors from cylinders. This practice resulted in a slight negative bias in detector response to the zero and span checks, as illustrated for one detector in Figure 8. Thus, because virtually all detectors exhibited a downward drift between the beginning and ending calibration and because the use of bags for zero and span checks resulted in a negative bias in detector response, the control limits used as criteria for recalibration were stricter than intended. Thus, detectors may have been recalibrated in selected cases when calibration was not necessary. However, the only impact of extra calibrations, if any, would be a minor improvement in accuracy.

The analyzer used to quantitate SF_6 concentrations for calculation of air infiltration rates was also included in the external performance audit. Based on audit concentrations ranging from zero to 800 parts per billion (ppb), the regression of analyzer response on audit concentration resulted in a slope of 0.94, an intercept of 7.2, and a correlation coefficient of 0.999. The average difference between audit concentrations and analyzer responses was 5.5 percent. Based on initial and final calibrations surrounding the period of investigation, instrument drift was negligible; initial and final slopes were 1.02 and 0.99, and initial and final intercepts were 4.1 and 6.5. At a calibration concentration of 400 ppb, the midpoint of the analytical range of the instrument, accuracy was +1 percent for the initial calibration and +2 percent for the final calibration; precision at the 400-ppb concentration was ±1 percent. Thus, the performance of the SF_6 analyzer also was well within data quality objectives.

Table 9. Changes in Slopes and Intercepts Between Beginning and Ending Calibrations for CO Detectors Used in the Investigation

Detector	Beginning calibration (11-30-87)		Ending calibration (12-7-87)		Change in slope, percent	Change in intercept, ppm
	Slope	Intercept	Slope	Intercept		
#037	0.99	0.26	0.99	0.13	0.0	-0.13
#104	0.97	0.48	0.97	-0.23	0.0	-0.71
#108	0.98	0.13	1.05	-1.21	+7.1	-1.34
#119	0.99	0.11	0.92	0.36	-7.1	+0.25
#123	1.01	0.10	0.99	-0.59	-2.0	-0.69
#130	0.98	0.45	0.99	-0.21	+1.0	-0.66
#142	1.01	-0.11	1.05	-0.41	+4.0	-0.30
#147	0.99	0.41	1.01	0.26	+2.0	-0.15
#153	0.99	0.04	0.99	-0.14	0.0	-0.18

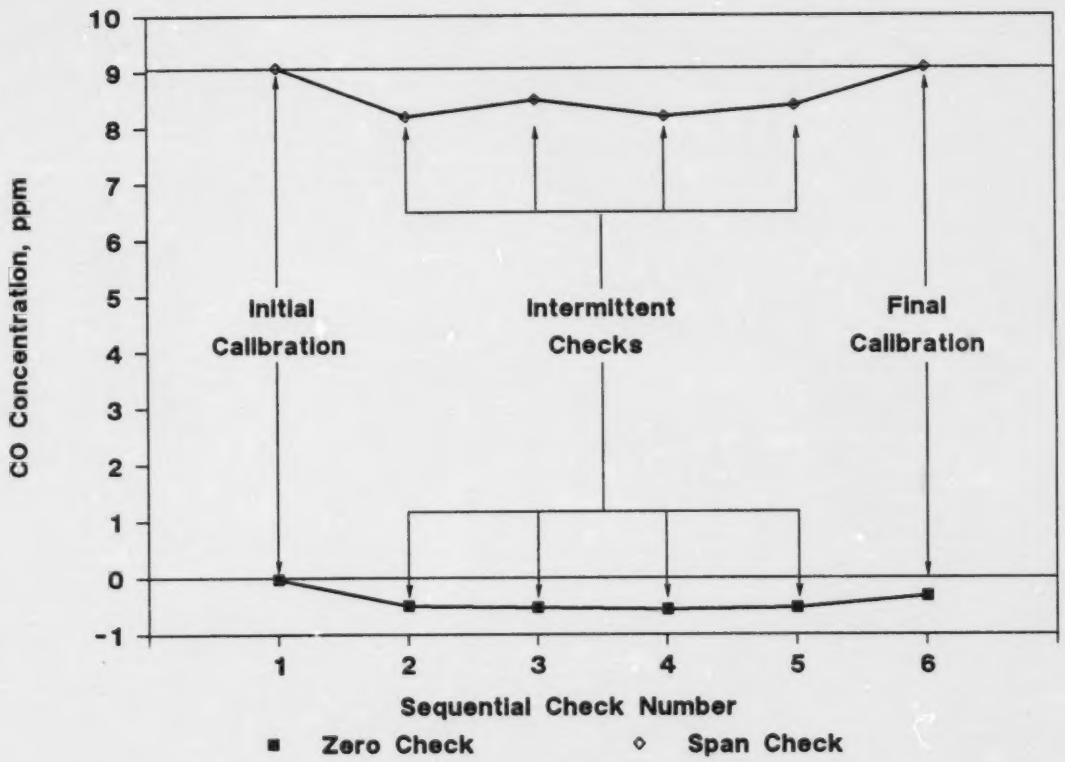


Figure 8. Response of one CO Detector to 0 and 9.06 ppm during multipoint calibrations and daily zero and span checks.

A representative subset of thermistors used to measure room air temperatures was also included in the performance audit. Of the 12 room thermistors audited, 8 differed from the audit reading by less than 0.5°F, two differed by less than 2°F, and 2 failed to meet data quality objectives. The two thermistors that failed were immediately replaced, prior to this investigation. Subsequent checks have verified proper performance of all thermistors in use at the research houses.

All meteorological instrumentation exhibited satisfactory performance during the audit except the windspeed/direction sensor. Windspeeds measured by the onsite sensor were low due to bearing wear. The unit was returned to the manufacturer for maintenance and calibration prior to this investigation, and additional quality control procedures were implemented to verify proper performance.

3.3. Concentration Profiles

This section summarizes basic patterns from the detailed monitoring network that reflect mixing and transport of the CO tracer. For each experiment, the monitoring points in the sampling plane were first treated as three vertical strips to examine trends in the vertical, and were then recompared by viewing the data as three layers to examine horizontal trends.

3.3.1. Room of Release

In the room of release, tracer concentrations at all six points began to rise rapidly very soon after tracer release was initiated and continued to climb as the tracer release was terminated (the end of the release period, 1.25 hours after the start, is indicated by a vertical line in Figure 9 and in subsequent figures). Peak concentrations were reached shortly after the source was turned off and then declined smoothly.

As shown in Figure 9, transport through the open doorway to the anchor string in the hallway was fairly rapid; concentrations at the anchor string rose and fell on essentially the same timing as in the room. Concentration gradients persisted during the release. At vertical string S_2 (between the release point and the doorway), concentrations were highest near the floor. At vertical string S_3, concentrations were highest near

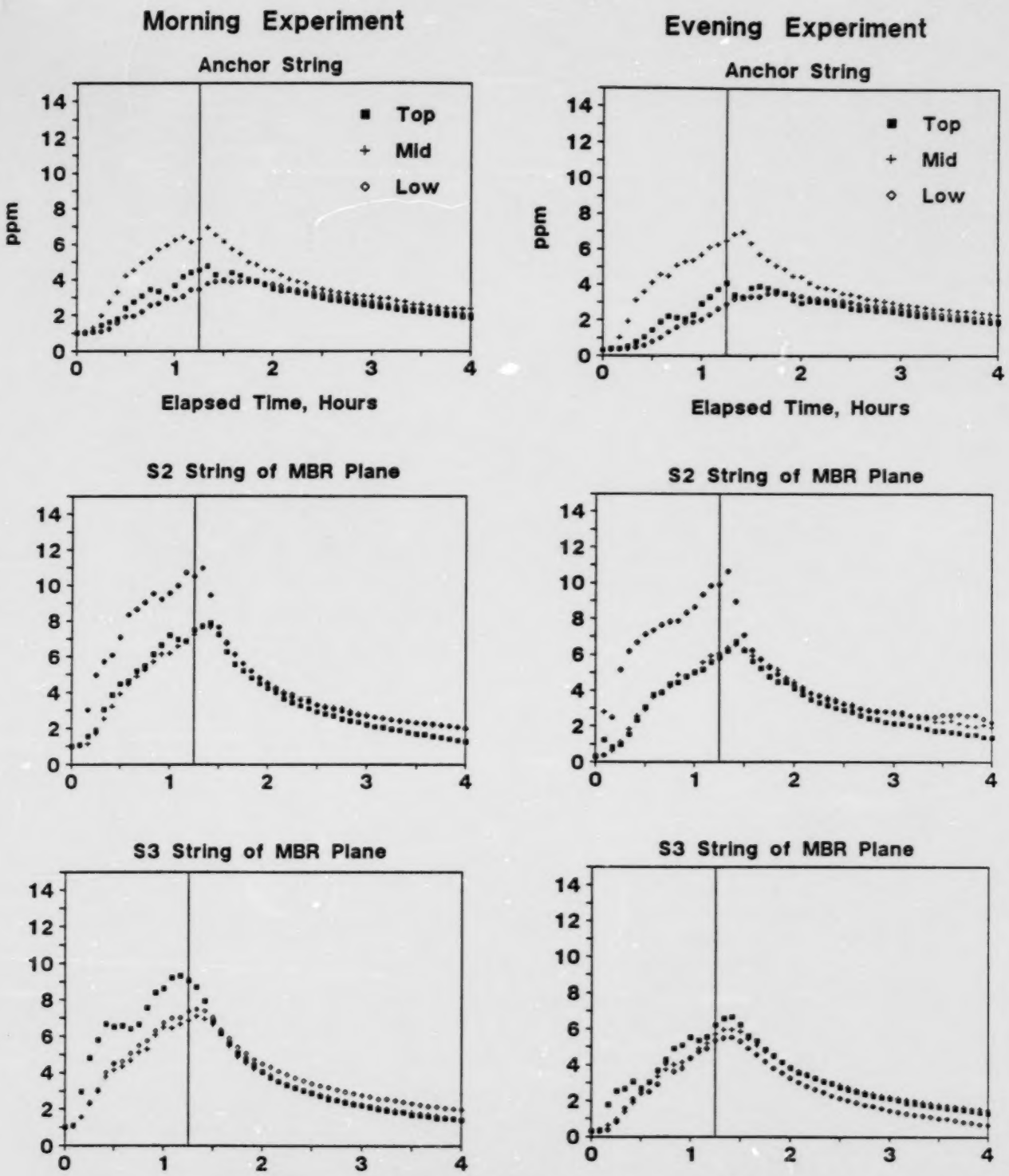


Figure 9. Vertical concentration gradients with CO detectors arrayed in the master bedroom.

the ceiling. At the anchor string, the highest concentrations occurred at midlevel. This pattern may be due to convective transport in the master bedroom. The temperature network, however, is insufficiently detailed to fully quantify such effects on thermodynamic grounds.

When the data were recomposed to form horizontal layers (Figure 10), the situation became clearer. Concentrations in the middle layer (1.2 meter height) at the two strings in the room and at the anchor string in the hallway were remarkably similar, rising and falling in unison and showing essentially the same pattern for the morning and evening experiments.

Convective circulation in the room of release could lead to uneven transport in the room of release, creating and sustaining concentrated packets that are slowly mixed into the general volume. In the top and bottom layers, where highest concentrations occurred in the room during tracer release, concentrations were as much as 40 percent higher than in the middle layer. Once the source was turned off, concentrations were rapidly equalized in the room. Vertical gradients, however, were sustained at the anchor string in the hallway for at least an hour after the source was turned off, and substantial differences persisted in the top and bottom layers between the room of release and the anchor point.

Although concentration profiles in the room of release appear to be driven by convection, the pathways of transport within the room cannot be fully appreciated because the sampling plane only provides a two-dimensional section through a three-dimensional transport field. Many different plume configurations can be envisioned that would lead to the same concentration profiles. Nonetheless, the following insights can be drawn from the perspective of mass balance modeling: (1) mixing proceeded rapidly in the horizontal and slowly in the vertical under conditions of natural air motions; and (2) in the room of release, convective motions created and sustained concentration gradients that led to poorly mixed conditions while the source was active. Concentration gradients in the room of release dissipated rapidly once the source was turned off.

3.3.2. Transport to Adjacent Rooms

Concentration profiles for the vertical sampling strings erected inside the doorways of rooms that adjoin the room of release are shown in Figure 11. Vertical gradients were largely dissipated by the time contaminants reached the D_2 string in the corner bedroom and the D_3 string in the front bedroom. Peak concentrations were substantially lower than in the room of release, and concentration profiles were delayed by approximately

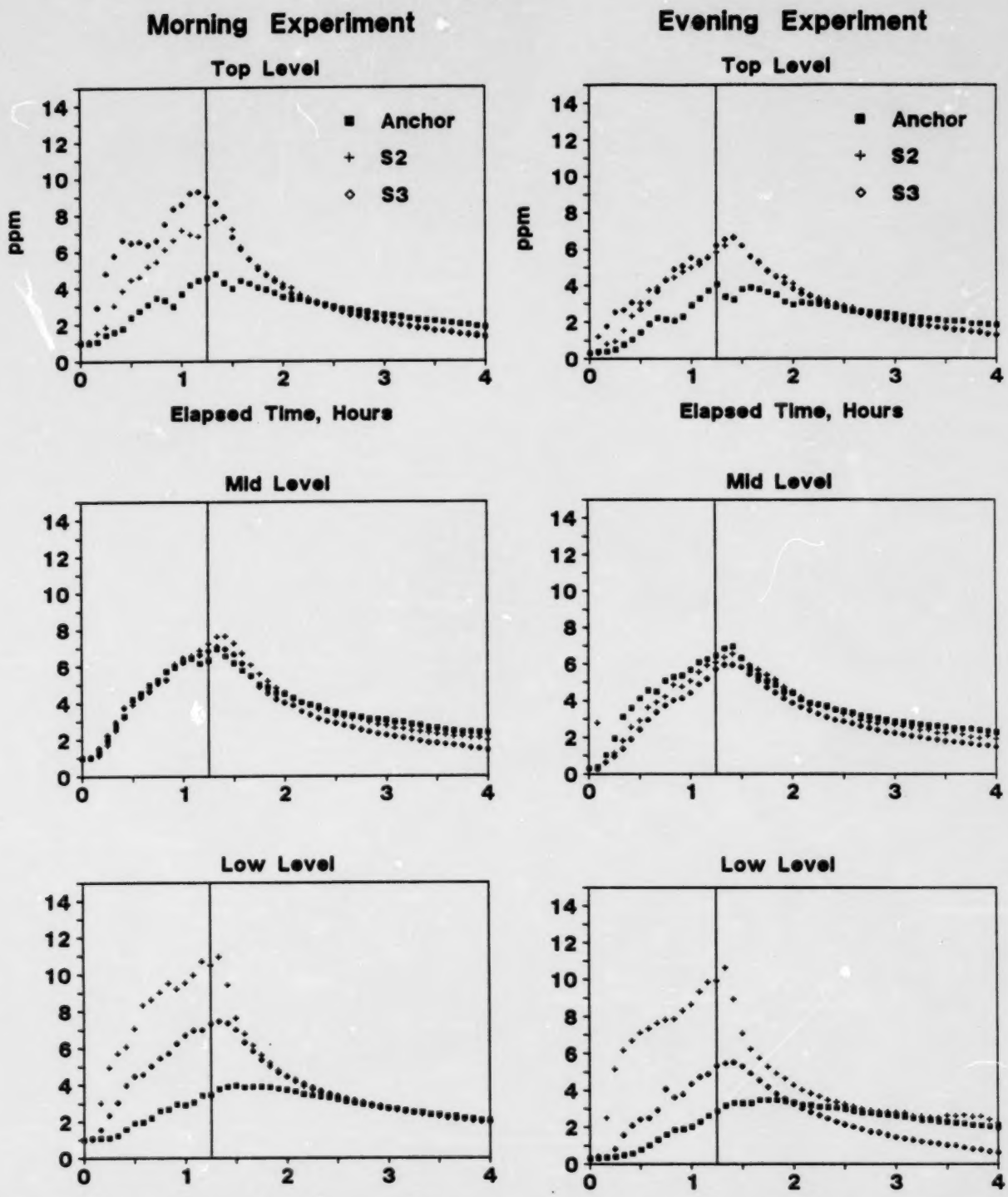


Figure 10. Horizontal concentration gradients with CO detectors arrayed in the master bedroom.

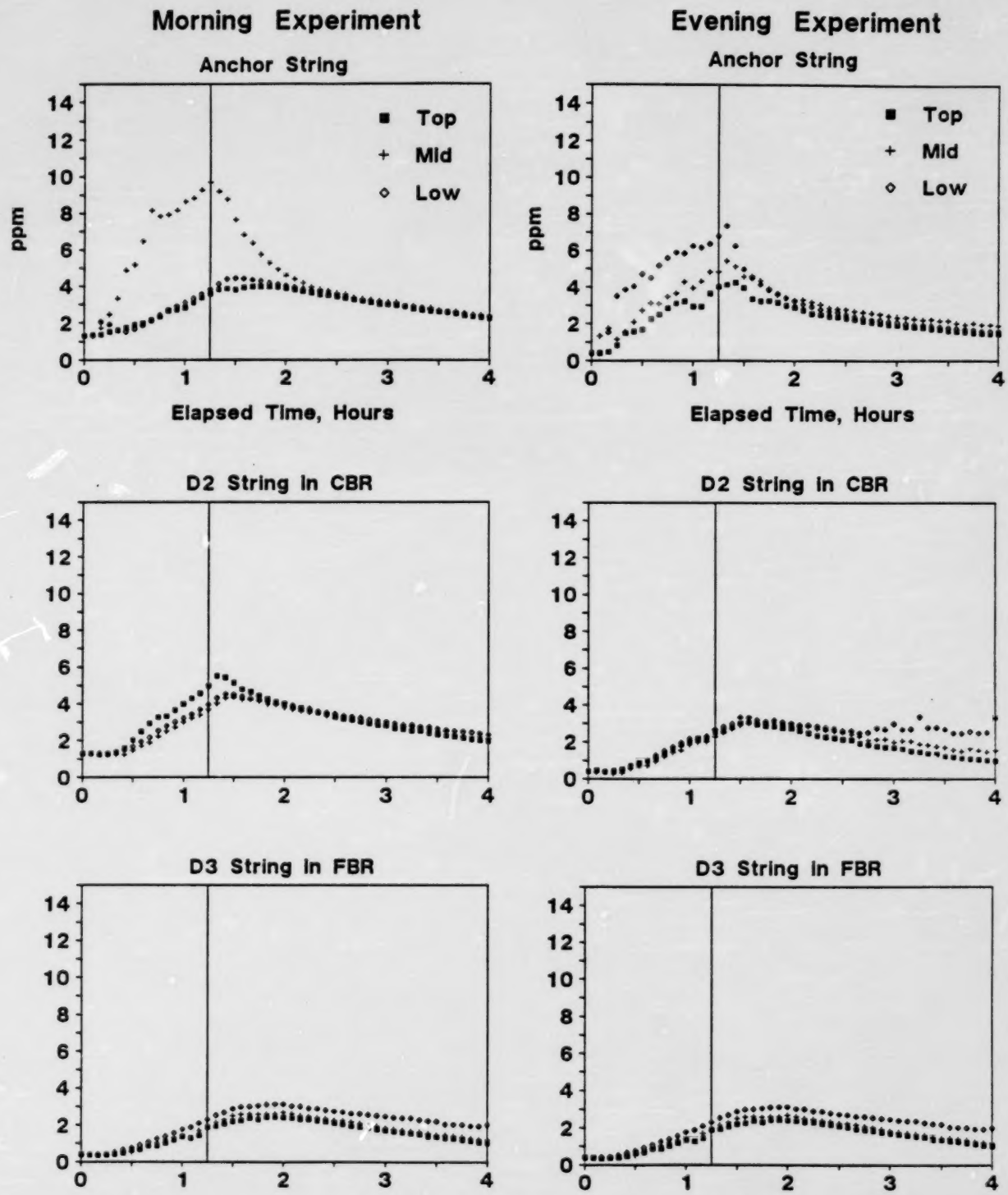


Figure 11. Vertical concentration gradients with CO detectors arrayed in adjacent bedrooms.

30 minutes and flattened. For the evening experiment, concentrations in the bottom level at the anchor string were higher than at the mid and top levels; this was the only experiment that deviated from the basic pattern of higher concentrations at the midlevel anchor.

Significant horizontal gradients persisted in the middle layer between these two rooms and the anchor point. As shown in Figure 12, midlevel concentrations were higher at the anchor for as long as an hour after the source was turned off. During the morning experiment, concentrations in the lower layers of the two bedrooms rose and fell in unison, suggesting strong coupling in the lower layer and rapid mixing within the two rooms.

During the evening experiment, horizontal gradients between the bedrooms and the anchor point were sustained at all levels for nearly an hour after the source was turned off. Nonetheless, the concentration profiles in both bedrooms were very similar to each other and to profiles from the morning experiment.

The following insights can be drawn from these two experiments: (1) contaminant transport into the adjacent bedrooms was primarily through the lower layers; and (2) mixing within these rooms was fairly complete and rapid.

3.3.3. Transport Through the Hallway

Concentration profiles for the vertical sampling strings erected along the hallway are shown in Figure 13. Vertical concentration gradients were evident for essentially the entire 4-hour period at the H_2 string (midway down the hall) and at the H_3 string (just past the foyer). By the time the contaminant transport reached the H_2 string, the highest concentrations were found near the floor. Concentrations at the H_2 string were consistently lower than at the anchor string. At the H_3 string, concentrations were even lower and more nearly homogeneous in the vertical.

Regular pulsations were strongly evident in these concentration profiles that did not prevail in the two bedrooms, supporting convective coupling of the hallway and living area, possibly including the basement zone through the stairwell. Recomposing the data to layer form (Figure 14), it is apparent that for the evening experiment the oscillations in the middle layer after the

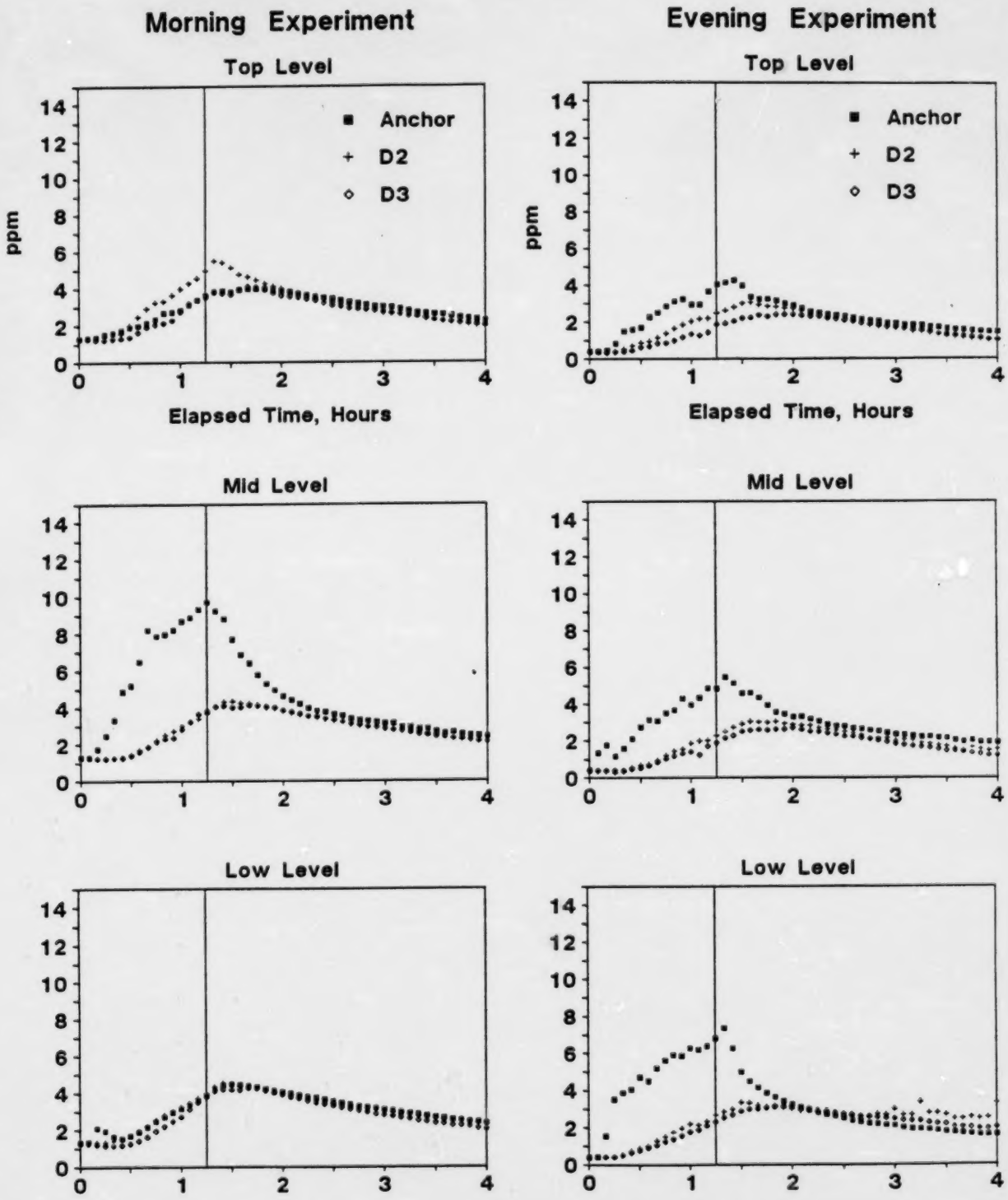


Figure 12. Horizontal concentration gradients with CO detectors arrayed in adjacent bedrooms.

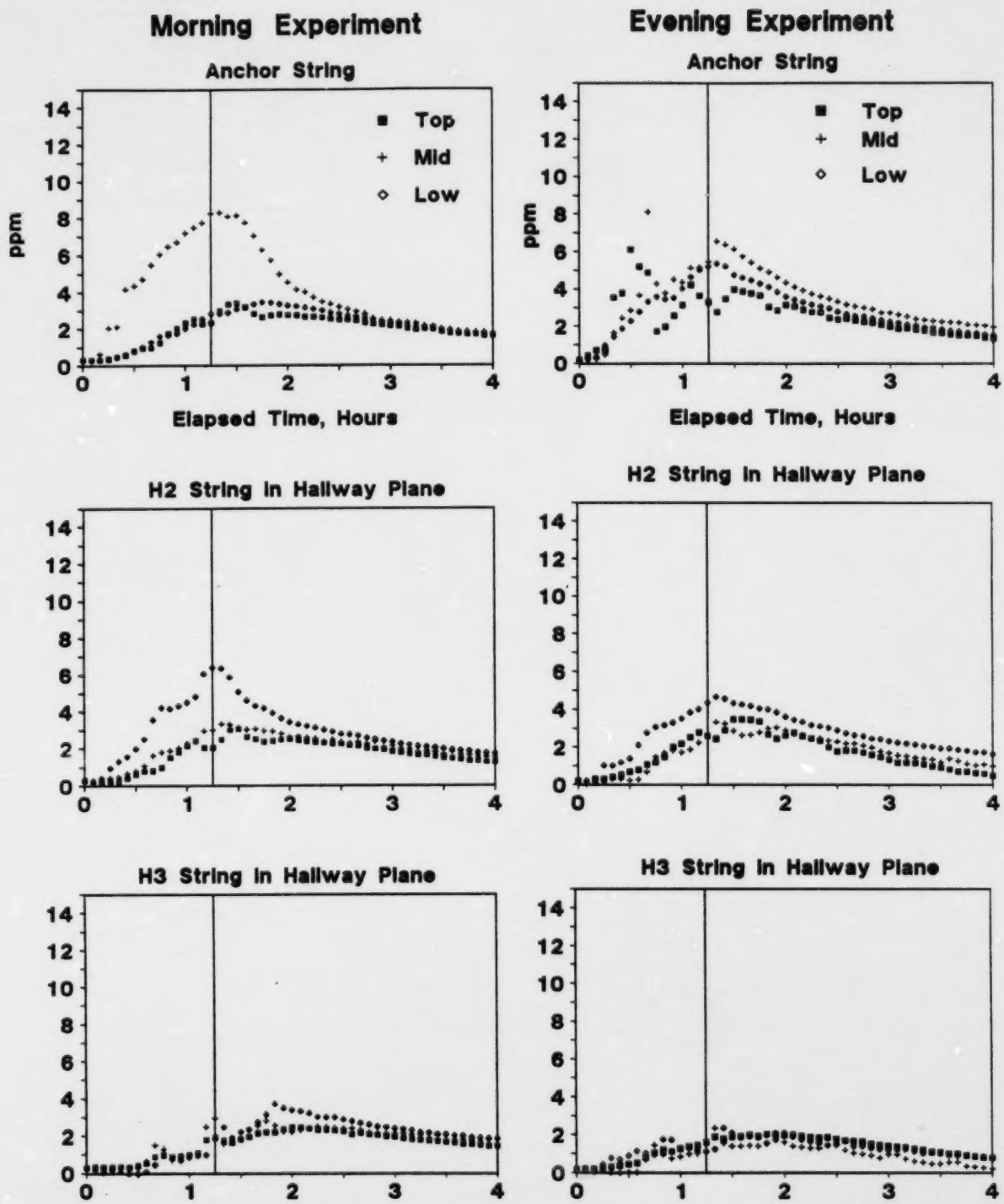


Figure 13. Vertical concentration gradients with CO detectors arrayed in the hallway.

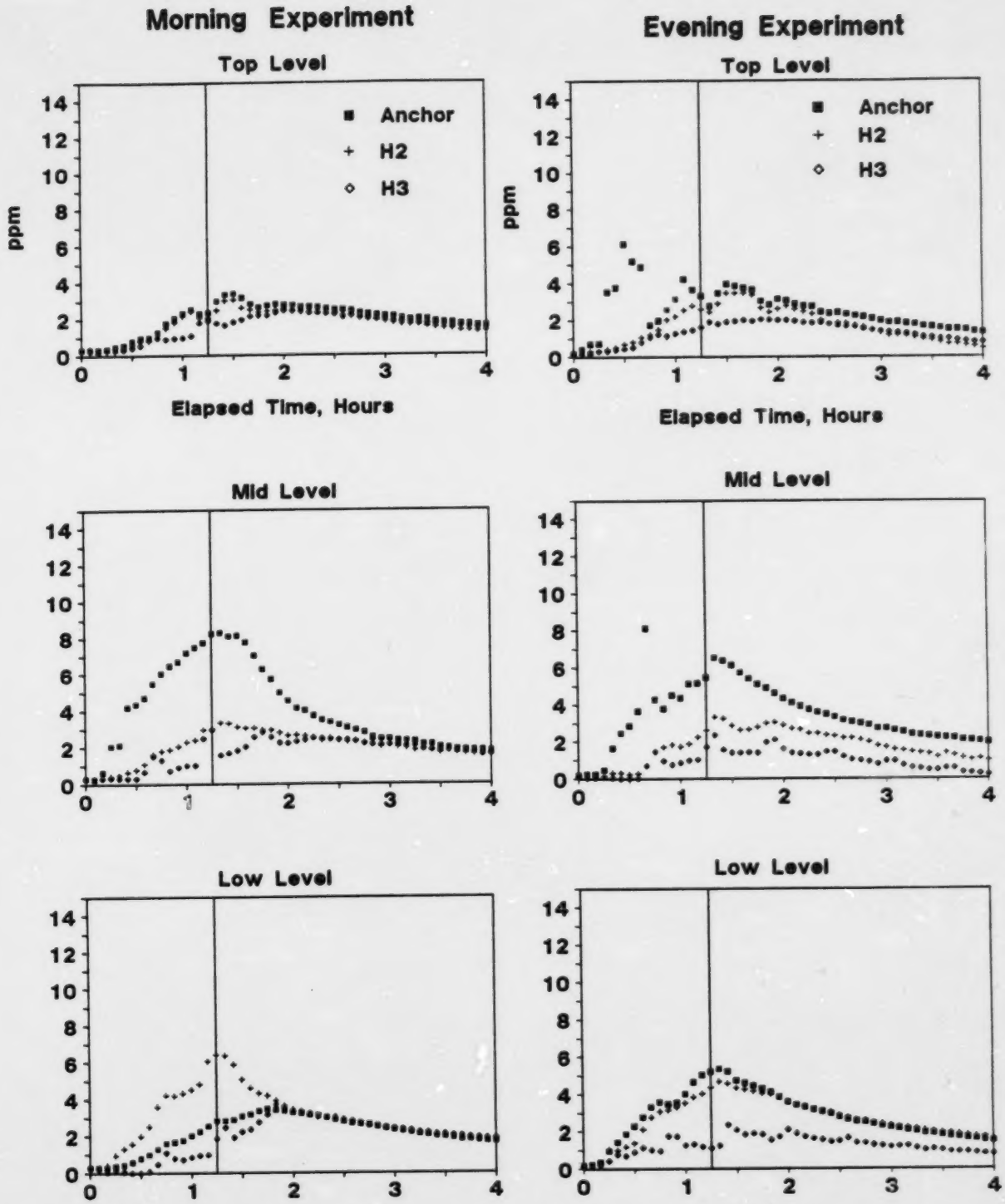


Figure 14. Horizontal concentration gradients with CO detectors arrayed in the hallway.

source had been turned off were parallel and extended from the living area (H_3) to at least midway down the hall (H_2), but were not reflected in the middle layer at the anchor string. These oscillations were faintly reflected in the top layer at the anchor and at H_2, suggesting general downturn. Strong convective action reflected in the middle and top layers at the anchor string was not coupled to profiles at the H_2 or H_3 sites.

During the morning experiment, concentration profiles were much smoother. Although some oscillations were evident, vertical gradients were dissipated fairly slowly but smoothly at all three sites, while horizontal gradients in the bottom and top layers dissipated within 30 to 45 minutes. In the middle layer, horizontal gradients between the hallway sites largely disappeared within an hour, but did not equilibrate with the anchor position until nearly 2 hours after the source had been turned off.

The following general insights can be drawn from these experiments:

- Concentrations in the hallway were lower than at the anchor site;
- Although vertical gradients were weaker in the hall, some stratification existed with highest concentrations prevailing near the floor; and
- Convective motions in the hallway provided fine structure to the concentration profiles.

3.4. Integration Across Experiments

To view experimental results in terms of active and passive exposures, unification of the three basic experimental types is needed for synthesis of a general case linking the room of release, adjacent rooms, and the remainder of the indoor volume. The main elements that enable this integration of results are the repetitive features of the experimental design.

In addition to strict repetition of time-related elements such as release rate and duration, the experimental design featured a stationary monitoring network to measure CO concentrations at three heights at the anchor site, at midlevel heights at four other indoor locations, and outdoors. As previously illustrated

in Section 2.5 (Figure 7), each vertical sampling plane provided a series of intermediate sampling sites connecting the anchor point to each of the fixed monitoring points on the main floor of the research house and to the room of release.

The research house itself represents perhaps the most powerful point of integration across the experiments in that it is a realistic full-scale model responding to changing environmental conditions; thus, the primary differences among validated data from experiment to experiment are traceable to naturally occurring changes in transport and mixing patterns. Although this features does not necessarily lead to a simple equivalence for uniting all experiments, it nonetheless presents additional information on the range of variability that prevails under real-world conditions.

Data integration across experiments was carried out from three perspectives:

- For each height level at the anchor location;
- At the midlevel height for the anchor location plus the stationary network; and
- At the midlevel height for the anchor, stationary network, and mobile sampling locations.

Concentration profiles at the anchor point are compared across all experiments in Figure 15. At the midlevel of the anchor, which was strongly associated with events in the room of release as well as in the adjacent rooms, peak concentrations varied by nearly a factor of 2 across all experiments but rose and fell in very similar fashion. This pattern indicates that similar forces were at work, but at different intensities. The highest peak concentrations in the middle layer were associated with morning experiments when convective coupling would be assisted by solar gains. During the concentration decay period following the end of CO tracer release, concentrations at all levels converged to a fairly narrow interval.

When attention is shifted to the mid-height of the anchor string in relation to the rest of the stationary monitoring network (Figure 16), it can be seen that additional factors came into play. Well-mixed conditions were usually approached within an hour after the release was turned off, but concentration

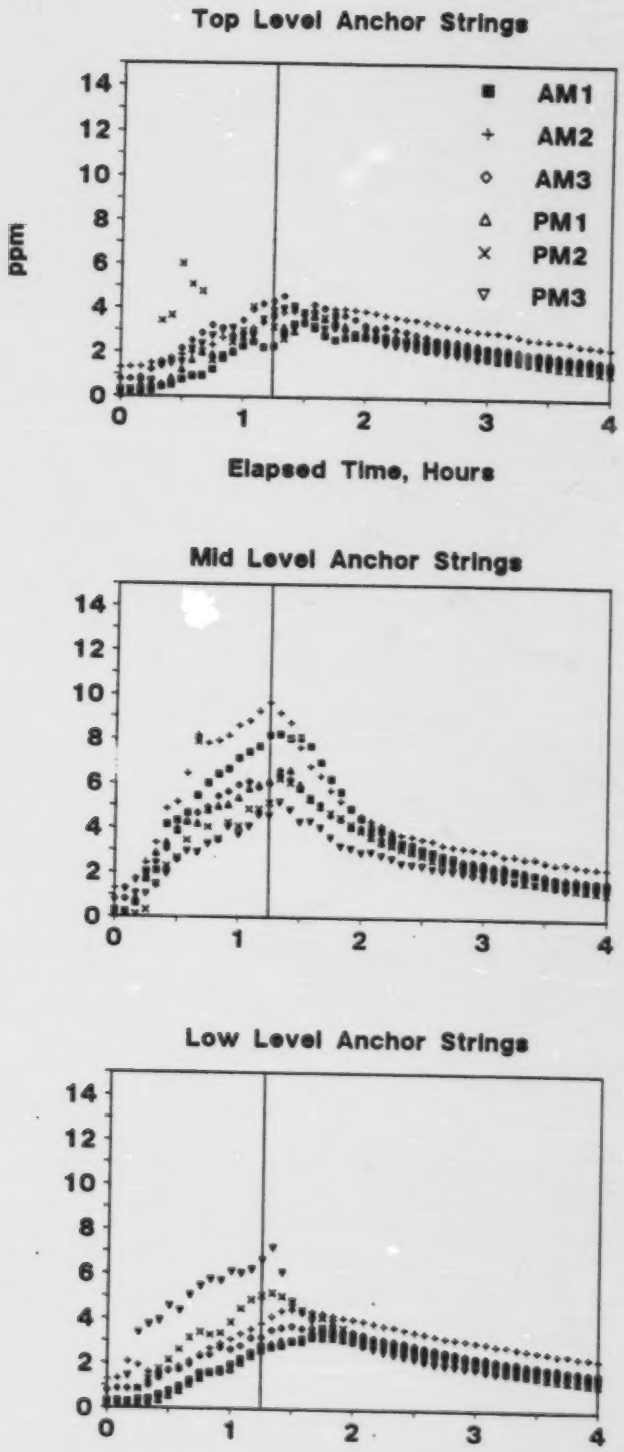


Figure 15. Concentration profiles across all experiments at the anchor point.

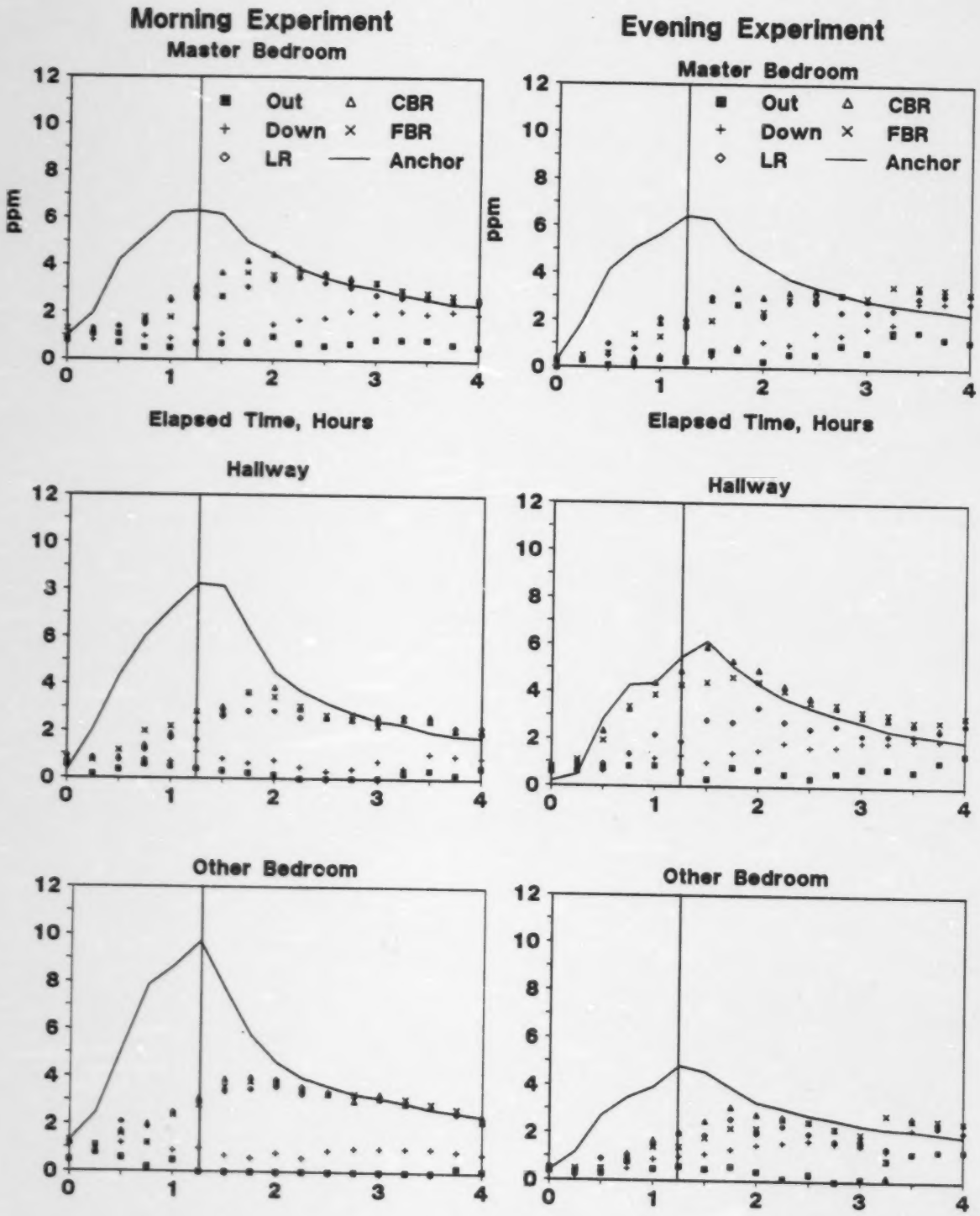


Figure 16. Concentration profiles for each experiment at the midlevel anchor point in the hallway and stationary monitoring sites.

profiles were sometimes affected by transport to the basement and, during some of the evening experiments, by infiltration of outdoor CO concentrations from mild outdoor peaks due to local traffic. There generally was greater separation between upstairs and downstairs concentrations during morning than evening experiments. Concentrations during the release period generally rose much more quickly at the anchor site than at any other location. The single exception to this trend was an evening experiment during which concentrations in the corner and front bedrooms rose nearly in unison with those at the anchor.

To develop characteristic concentration profiles connecting all measurements taken in the middle layer of the main floor, the data sets were combined in three stages. First, site-specific averages across all experiments were constructed for each location that was common to all experiments (i.e., midlevel anchor and the stationary network). Second, data from the midlevel of the vertical sampling strings that were relocated from experiment to experiment were normalized as a fraction of the corresponding midlevel anchor concentration at the end of the release period for each experiment. Third, the normalized values were multiplied by the grand-average midlevel anchor value at the end of the release period to rescale the normalized data in terms of average conditions.

Concentration profiles obtained through this exercise were examined as 15-minute snapshots. Throughout the release period (Figure 17), concentrations in the room of release and at the anchor point in the nearby section of the hallway were virtually identical. Concentrations tapered off substantially beyond the anchor point, such that noticeable increases in the other bedrooms and living room were not evidenced until 45 to 60 minutes after the release was started. Mixing within the adjoining bedrooms appeared to be rapidly achieved, as indicated by very similar concentrations near the doorway and center of each room.

Following the release period (Figure 18), spatial uniformity throughout the house was nearly achieved as concentrations in the release area receded and concentrations in other areas continued to rise. In particular, within 60 minutes after the release period ended, concentrations began to recede in all upstairs locations that were monitored, and concentrations in likely receptor locations (each bedroom and the living room) were within 0.6 ppm of one another. Further unification of experimental results and contaminant migration patterns can be obtained through modeling efforts presented in the next section.

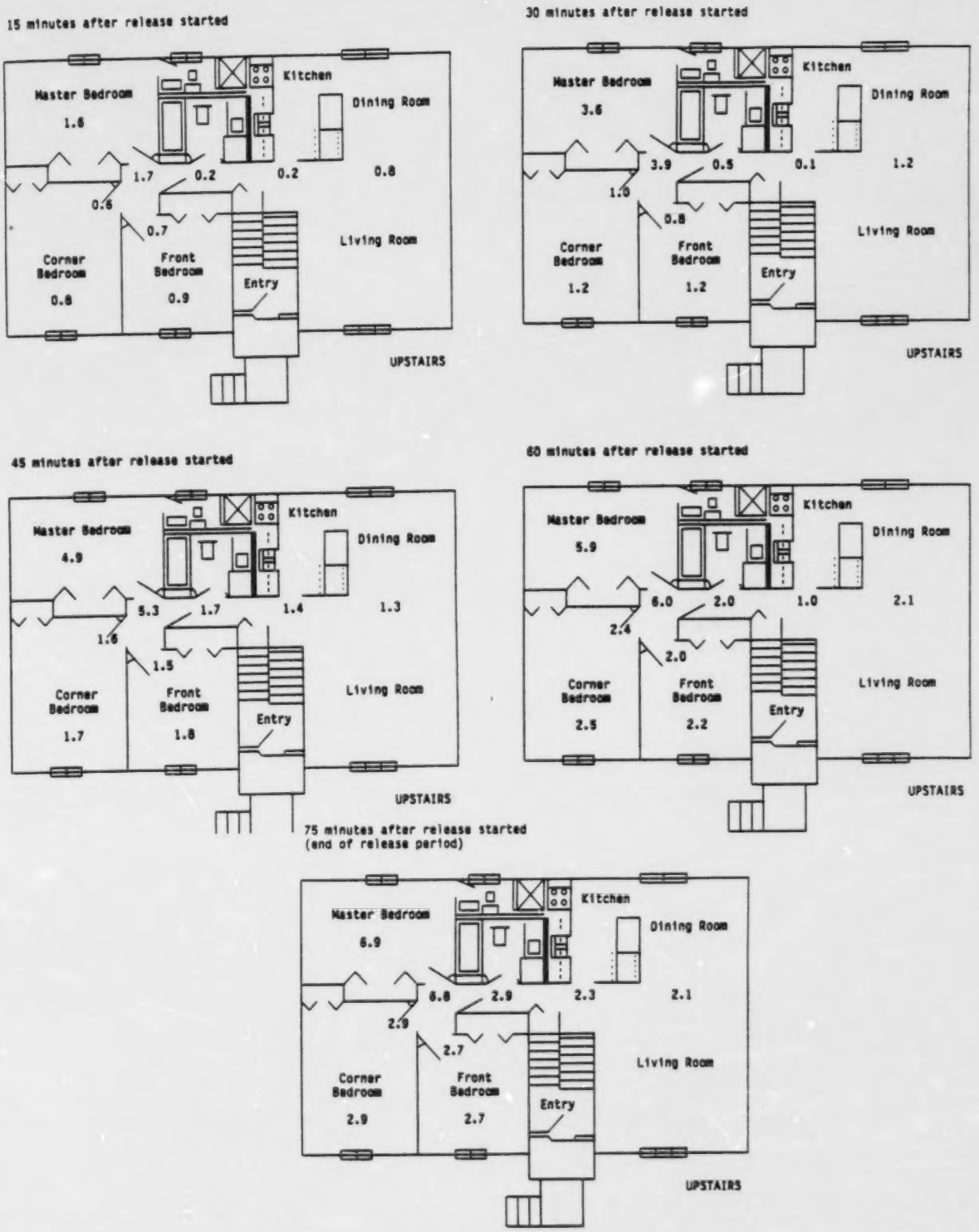


Figure 17. Spatial profile of CO concentrations (in ppm) upstairs during the release period.

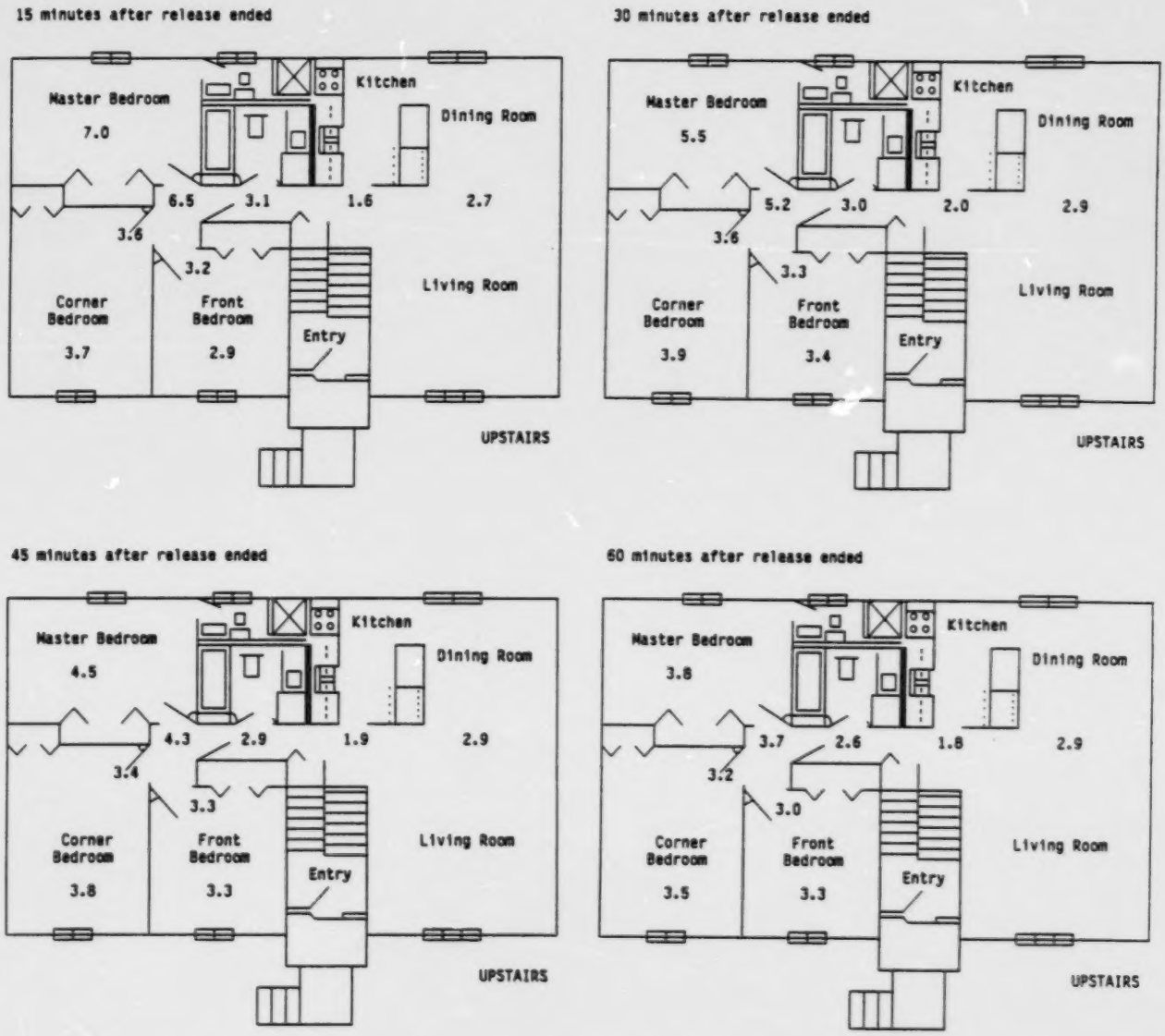


Figure 18. Spatial profile of CO concentrations (in ppm) upstairs following the release period.

4. ANALYTICAL MODELING

The practical objectives of the work reported here involved (1) examining advantages and limitations associated with simplified mass balance modeling of complex scenarios and (2) identifying avenues of useful improvements through multichamber modeling. Modeling activities began with the generalized single-chamber mass balance model, using inputs of air exchange, source rates, and indoor volume. Multichamber modeling, using interzonal airflows from previous PFT measurements analyzed by Brookhaven National Laboratory (BNL), was then carried out to identify improvements resulting from this next level of model complexity.

4.1. Single-Chamber Mass Balance Model

The single-chamber mass balance model (see Appendix A) was run on a 15-minute time step to calculate indoor concentrations at time intervals consistent with averaging periods for the stationary monitoring network. Separate calculations were performed at air exchange rates of 0.2, 0.3, and 0.4 air changes per hour (ACH) to cover the range of air infiltration rates that occurred during the experimental period. All model calculations assumed perfect mixing and negligible outdoor levels.

As shown in Figure 19, peak concentrations under nominal conditions coincide with the end of CO tracer release and occupy a fairly narrow concentration interval, ranging from 3.2 ppm for the 0.4-ACH case to 3.6 ppm for the 0.2-ACH case. By the end of the experimental period, the dilution effects of the different levels of air exchange decrease concentrations by half while broadening the differences between cases.

The single-chamber model, when applied to the general air volume of the main floor of the research house, significantly underpredicts peak concentrations observed in the room of release and at the anchor point. Figure 20 illustrates this lack of correspondence for a morning experiment. In this figure, concentration profiles from the middle levels at the anchor and S_2/S_3 (master bedroom) strings are plotted together with model estimates calculated at 0.3 ACH. The calculated peak concentration of 3.4 ppm falls short of measured values by a factor of 2, and the model does not approach measured values until near the end of the decay period.

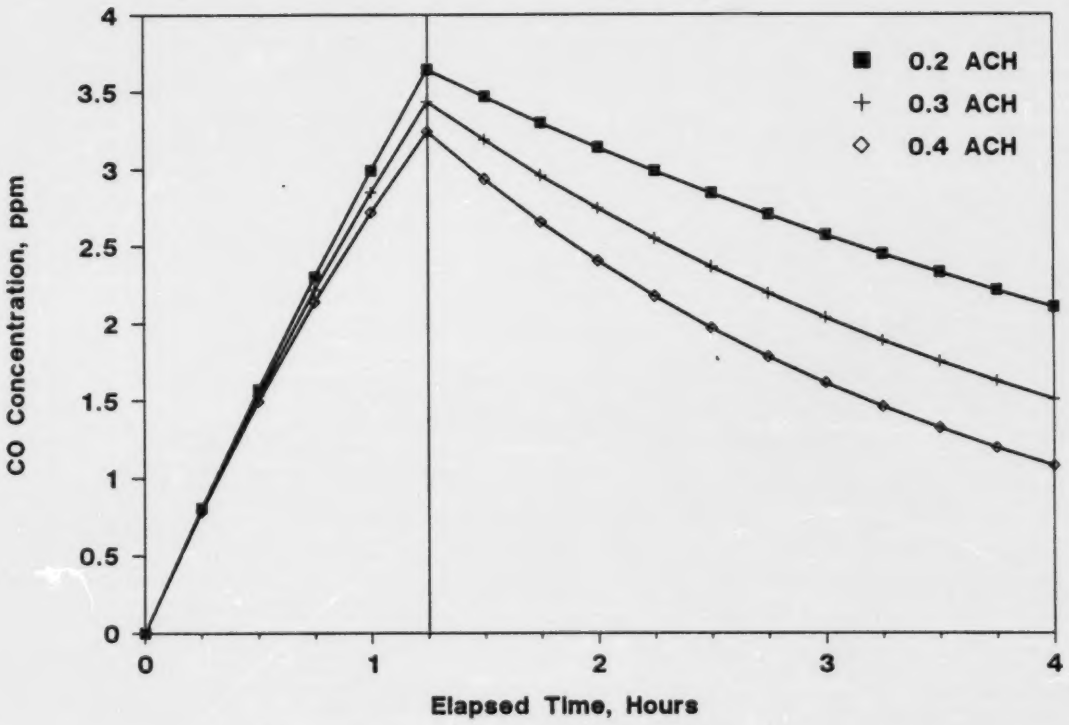


Figure 19. Single-chamber mass balance model calculations for generalized experimental conditions.

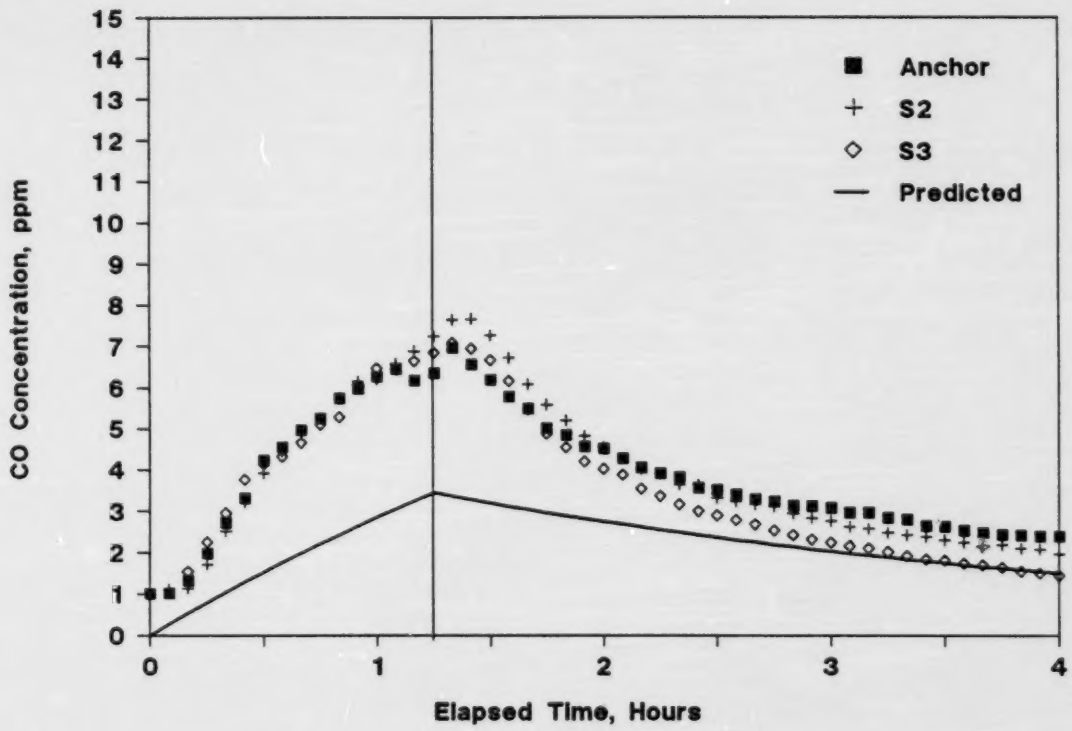


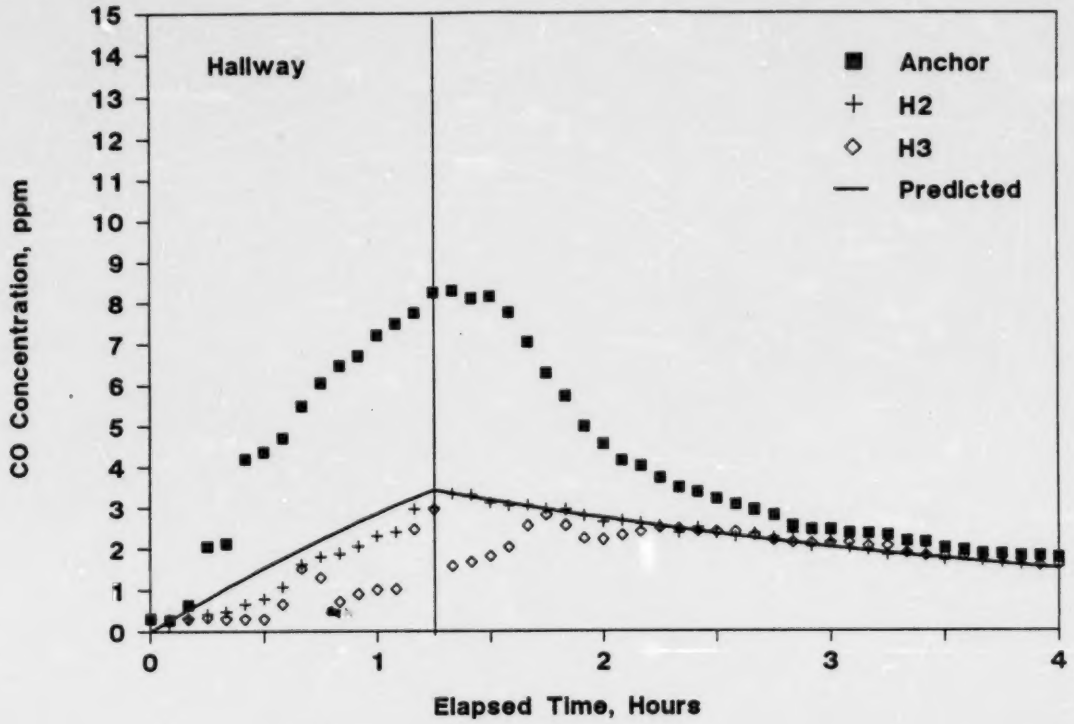
Figure 20. Comparison between single-zone model predictions and measurements near the release area (experiment type 1, morning run).

Comparisons at monitoring points that are distant from the release area, however, begin to show remarkable agreement. The concentration profiles for distant strings of the hallway plane (Figure 21, upper part) and the strings inside the doorways of rooms adjacent to the room of release (Figure 21, lower part) are largely reproduced by this simple model.

The primary shortfall of the model for areas distant from the release point lies in the relative timing of peak concentrations. Modeled peak concentrations occur at the end of the tracer-release period. At the midlevel of the hallway, the measured peak at the H_2 string, midway down the hall, occurred 5 minutes after the release ended. At the far end of the hall (the H_3 string), the peak occurred 30 minutes after the release had ended. At the D_2 and D_3 strings, located just inside the doorways of the second and third bedrooms, measured peaks occurred 10 minutes after the release ended. On the day of this experiment, ambient levels of CO were at approximately 1 ppm as the experiment began; although the outdoor concentration declined as the experiment progressed, the outdoor influence resulted in a slight offset that was not reflected in the model.

Figure 22 illustrates the correspondence between the nominal model case and 15-minute measurements from the stationary network. Although the model estimates at these points indicate an earlier occurrence of the peak concentration than do the measurements, the general correspondence is excellent.

The single-chamber mass balance model does not account for spatial gradients; it tracks the overall retention of the contaminant, providing estimates that correspond to volume-weighted averages. To examine this concept, volume-weighted average concentrations were calculated on a 15-minute basis using data from the stationary network and the midlevel probe of the anchor string. As shown in Figure 23, these volume-weighted averages are in good agreement with the nominal model case. Even though concentrations near the release are up to 4 times higher, they occupy only 20 percent of the total volume. The single-chamber mass balance, then, provides a fairly close approximation of general concentration profiles that relate to passive exposure, but tends to underestimate concentration profiles that relate to active exposure.



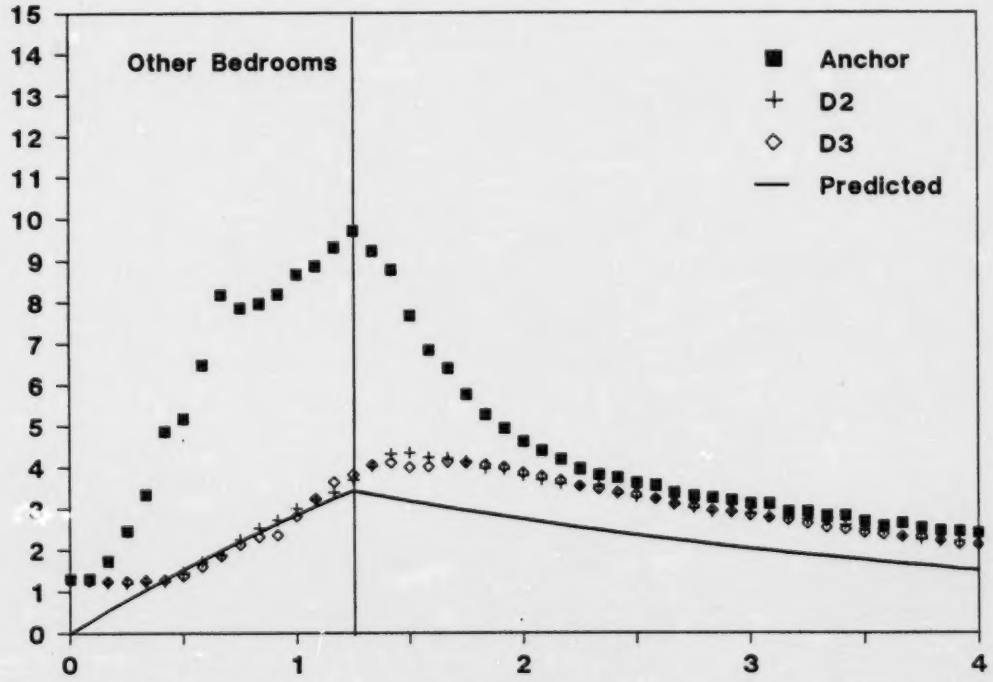


Figure 21. Comparison between single-zone model predictions and measurements in the hallway and front bedrooms (experiment types 2 and 3, morning runs).

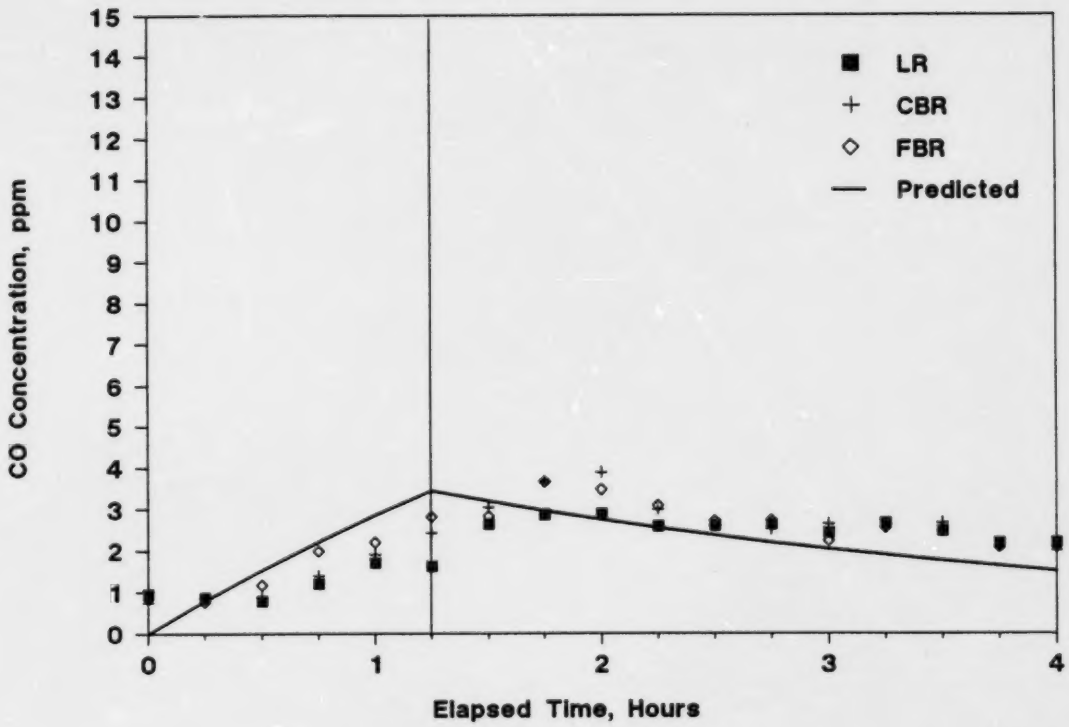


Figure 22. Comparison between single-chamber model predictions and measurements at stationary monitoring locations that represent likely sites of passive exposures (experiment type 2, morning run).

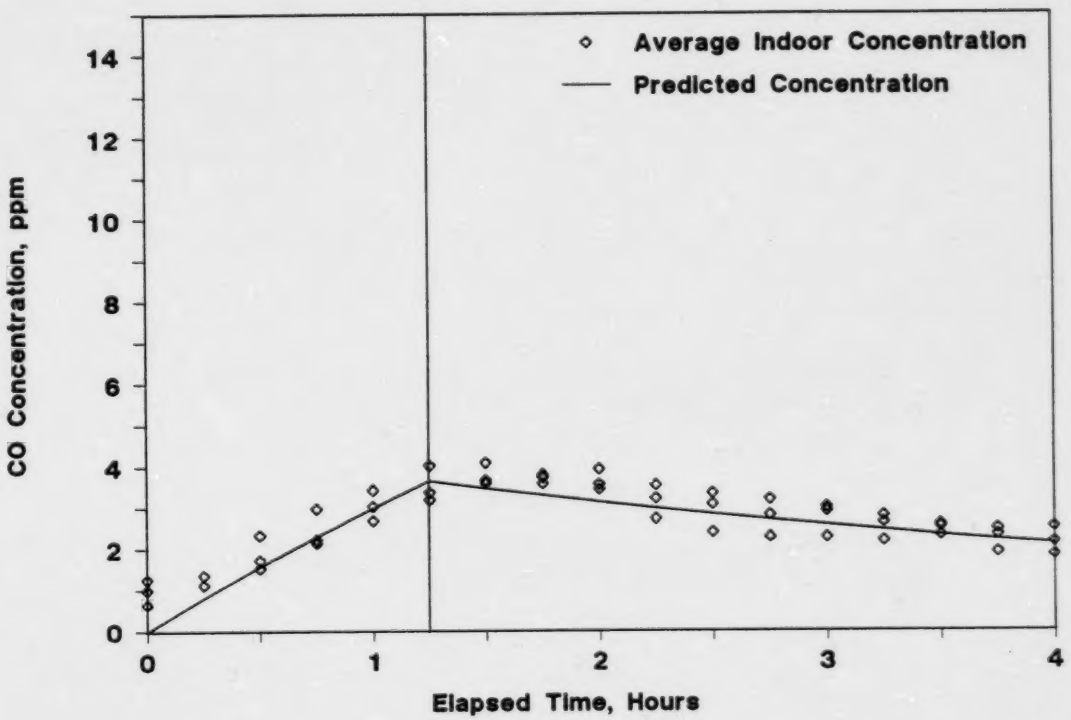


Figure 23. Comparison between single-chamber model predictions and volume-weighted average indoor concentrations for three morning experiments.

The single-chamber model cannot simultaneously estimate active and passive exposures with equal accuracy because the emissions are dispersed (in the model) to the general indoor air volume and are therefore equal throughout the house. From these experiments, it is obvious that there was both confinement in the room of release plus time-consuming transport to other rooms, resulting in the strong spatial and temporal differences that were observed.

In concept, the single-chamber model could be exercised twice, first using the volume of the release room to estimate active exposure and then using the general volume to estimate passive exposure. However, shrinking the reference volume to that of the release area (master bedroom) would result in overestimates of active exposure. For example, for these experiments, substituting the 40-m^3 volume of the master bedroom for the 215-m^3 volume of the main floor would increase peak modeled concentrations by the ratio of the volumes (5.4), producing peak concentrations near 20 ppm where approximately 10-ppm levels were observed; this discrepancy is due to the dilution effects of transport to other rooms.

There are two alternatives for increasing prediction accuracy--(1) developing empirical values to increase the effective removal rate of contaminants when using a single-zone model to estimate active exposure and (2) using a multichamber model to simultaneously estimate active and passive exposures. The second alternative--using a multichamber model--would seem to be a more natural and straightforward approach.

4.2. Multiple-Chamber Modeling

A two-chamber mass balance model was formulated using interzonal flows derived from previous PFT measurements at the research house. For this model analysis, the master bedroom was defined as zone 1 (volume of 40 m^3), and the living/dining area, hallway, and the two smaller bedrooms were treated as the second zone (volume of 175 m^3). Specific equations used in this analysis are presented in Appendix A. For this synthetic case, flow coupling between the upstairs and the basement was ignored. As shown previously (Section 3), CO tracer would be occasionally transported to the basement zone, but this occurrence did not significantly alter the general form of the concentration profiles upstairs.

The system of interzonal and infiltration/exfiltration flows used in the two-chamber model is illustrated in Figure 24. These airflows were directly adapted from PFT measurements that were taken over an 18-hour period in January 1985 at the research house. This particular set of PFT measurements was acquired to assess baseline conditions for experiments being conducted at that time. As with the experiments reported here, operation of the central circulation fan was suppressed. Interzonal airflows derived from the PFT data, although not necessarily equal to those that occurred during the experiments reported here, nonetheless provide characteristic values that are appropriate for model applications.

The two-chamber mass balance model provides substantial improvement in estimating active exposure, while retaining the good correspondence with passive exposures that was obtained with the single-chamber model. As shown in Figure 25, calculated peak concentrations reached 9.2 ppm in the master bedroom (zone 1) and 3.0 ppm in zone 2. Model calculations reproduce measured concentration profiles in the midlevel at both the anchor site and the far end of the hallway for the morning experiment when the vertical sampling plane was placed along the hallway.

Even though environmental conditions varied across experiments, the two-chamber model calculations, which are predicated on nominal conditions, provide good estimates of peak and average concentrations for all of the experiments. Table 10 summarizes the range of measured peak and average concentrations at key indoor locations, along with estimates from the single- and two-chamber models. The single-chamber model is in best agreement with measurements in the living area, and increasingly underestimates peak and average concentrations at locations that are closer to the release area.

For the two-chamber model, calculated peak and average concentrations for zone 1 are in the center of the observed range for the six analyzers situated in the master bedroom for one of the morning experiments. At the anchor site and other locations where measurements are available for all experiments, the two-chamber model passes through a transition phase where zone 1 estimates are overtaken by zone 2 estimates in terms of agreement with measured values. The anchor site represents perhaps the most important transition between the two defined chambers.

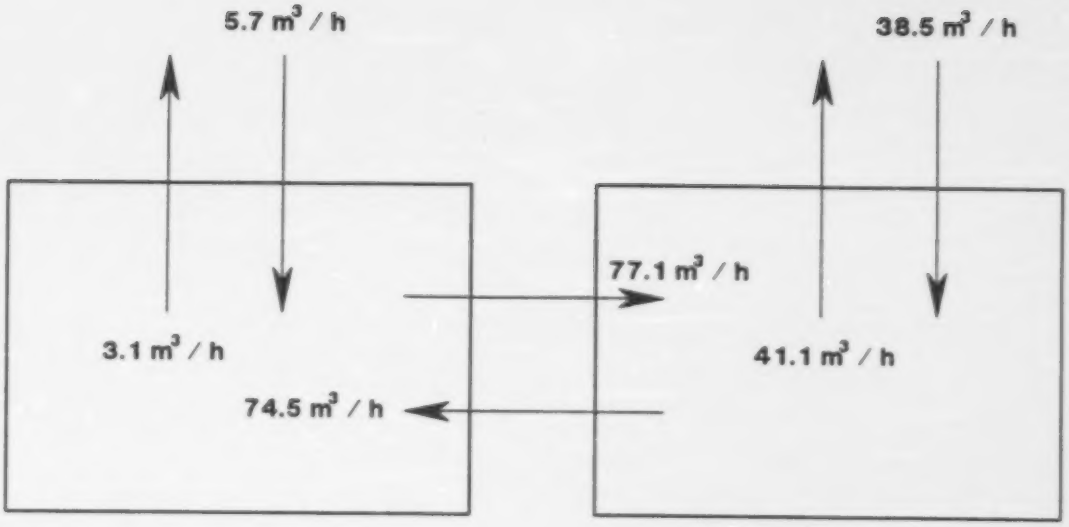


Figure 24. Airflows used as inputs to a two-chamber model.

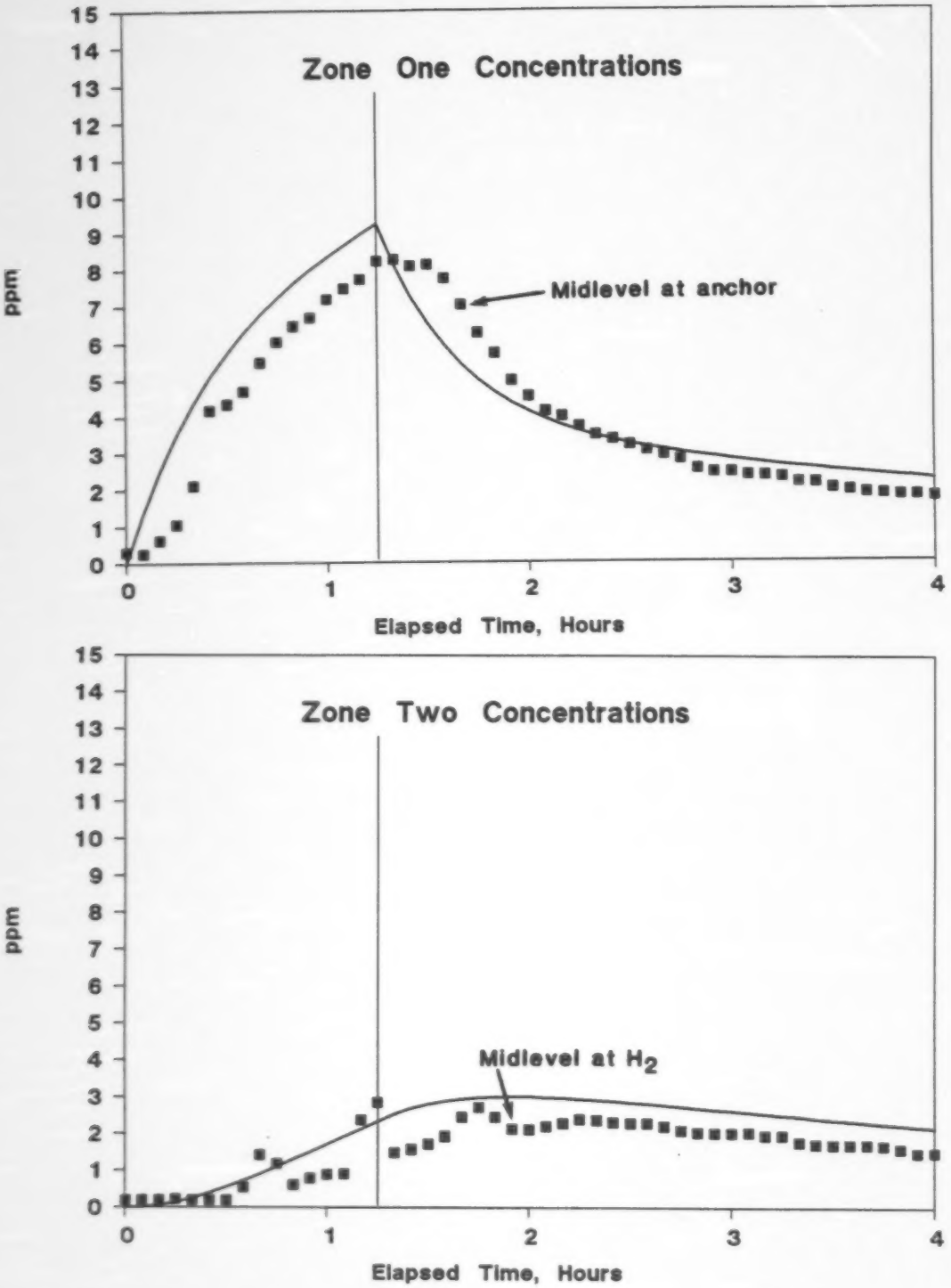


Figure 25. Comparison between two-chamber model predictions (indicated by a line) and measured concentrations in each zone (indicated by squares) for morning experiment type 2.

Table 10. Comparisons of Model Estimates and Measured Values for Peak and Time-Weighted Average Concentration During and After Contaminant Release

	Peak concentration (ppm)	4-h Average concentration (ppm)
MODEL ESTIMATES		
Single chamber	3.4	2.2
Two chamber--zone 1	9.2	4.5
Two chamber--zone 2	3.0	2.1
RANGE OF MEASURED VALUES		
Master bedroom	(7.1-11.0)[a]	(3.7-5.0)[a]
Anchor site--midlevel	6.3-8.2	3.8-4.7
Corner bedroom	3.9-4.5	2.3-2.9
Front bedroom	3.7-3.8	2.3-2.7
Living room	2.9-3.6	2.1-2.7

[a] Range of values from six sensors in one experiment; all others are range of values across all experiments.

In the two-chamber model, the anchor site would be assigned to the general air volume (zone 2) because it receives material from the release zone and is physically outside the master bedroom. However, as shown in Section 3, concentration profiles at the anchor site differed from the convective patterns in the master bedroom and from the well-mixed conditions that were approached in other rooms. Developing a separate volume centered on the anchor, supported by correcting flows to direct the transport to other rooms, would be an interesting avenue of possible refinement to the two-chamber model. Although such an approach would offer refinements in reproducing time-related events such as the delay to reach peak concentrations away from the release point, the physical justification for defining additional volumes requires additional information.

5. DISCUSSION

An overall perspective relating to goals and needs for assessment of consumer exposures is provided in Section 5.1. Major insights gained from this investigation and future actions that can be taken to fill specific types of information gaps are discussed in Section 5.2.

5.1. General Perspective and Needs

An important objective pertaining to OTS exposure assessments is to provide accurate estimates of active and passive exposures resulting from different patterns of consumer product use in residential environments. One means of meeting this objective is by developing a computer model that can provide accurate predictions of exposures for a wide variety of scenarios.

As indicated in Figure 26, a number of user inputs, table lookups, and computer calculations are needed to support a fully-specified computer model for active and passive exposures to emissions from consumer products used in residential environments. Many of the lookups and calculations go beyond the capabilities of the Computerized Consumer Exposure Models (CCEM) in current use but could be obtained through future data acquisition efforts.

In Table 11, vital inputs to model lookups and calculations are shown in relation to various types of data sources that currently exist or that could exist as a result of future data acquisition efforts. Four possible sources of data--results from chamber studies, consumer surveys, measurements with perfluorocarbon tracers (PFTs), and experiments in research houses--are indicated in the table; in addition, surveys in which contaminants released from consumer products are monitored in residential settings will also be needed to validate consumer exposure models. Alternative approaches for filling information gaps through chamber studies, consumer surveys, and monitoring surveys were discussed in a recent report (GEOMET, 1987c) that was prepared for EPA.

One of the most significant voids in current exposure assessments is the lack of appropriate values for air infiltration rates and interzonal airflows. As shown in Table 12, combining data from past PFT measurements and future research house experiments can substantially fill this gap. These two types of data sources are very complementary: PFT measurements cover a

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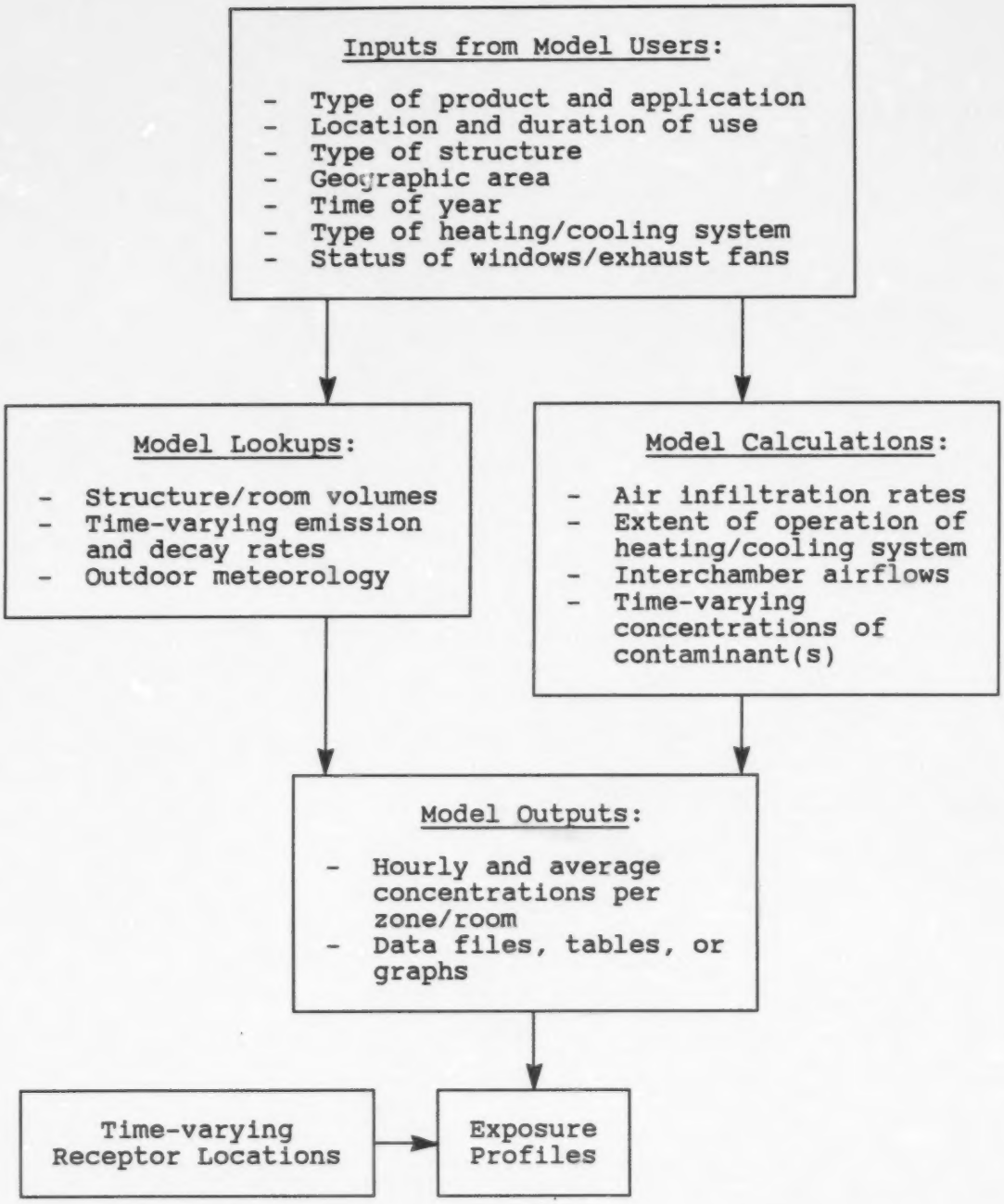

Inputs from Model Users:
- Type of product and application
- Location and duration of use
- Type of structure
- Geographic area
- Time of year
- Type of heating/cooling system
- Status of windows/exhaust fans
Model Lookups:
- Structure/room volumes
- Time-varying emission and decay rates
- Outdoor meteorology
Model Calculations:
- Air infiltration rates
- Extent of operation of heating/cooling system
- Interchamber airflows
- Time-varying concentrations of contaminant(s)
Model Outputs:
- Hourly and average concentrations per zone/room
- Data files, tables, or graphs
Time-varying Receptor Locations
Exposure Profiles

Figure 26. Overview of consumer exposure model.

Table 11. Important Inputs to Model Lookups and Calculations and Associated Data Sources

Type of input	Data sources			
	Chamber studies	Consumer surveys	PFT data base	Research house experiments
Emission rate				
- Duration/rate of use for various products		X		
- Emission rate specific to product and usage pattern	X			(X)
Decay rate	X			(X)
Volume/mixing/transport				
- Configuration and/or involvement of floors/rooms	(X)	(X)	(X)	(X)
- Extent of heating/ cooling system operation				(X)
Air exchange				
- Infiltration rate	X		(X)	(X)
- Ventilation rate		X		(X)
- Interchamber airflows	(X)		(X)	(X)

X = Some data already exist.

(X) = Data could be obtained through future acquisition/assimilation efforts.

Table 12. Utility of PFT Data Base and Research House Experiments

Characteristic	PFT data base	Research house experiments
Structure types and geographic areas	Various	Limited
Spatial coverage per structure	1 to 4 zones	Individual rooms
Weather conditions per structure	Limited	Various
Internal conditions per structure	Largely unknown	Various (can be controlled)
Resultant airflows	Average	Time-varying or average

broad array of geographic areas and structure types, but are limited in spatial, temporal, and operational details for each structure; by comparison, research house experiments provide much greater detail on temporal and spatial variations for various conditions of product use, but may have less generalizability. However, the transferability of results from research house experiments can be greatly aided by replicating selected experiments in other common types of occupied structures, such as apartments, townhouses, and selected configurations of single-family detached homes.

As noted in a recent scoping report (GEOMET 1987a) on the topic of room-to-room contaminant migration, a relatively rich repository of data concerning time-averaged air infiltration rates and interzonal airflows for a variety of structures and geographic areas is currently maintained at Brookhaven National Laboratory. The analytical potential of these data cannot yet be exploited because the results are not fully unified in a computer-accessible format, but efforts toward this end have begun. Such efforts, coupled with future research house experiments, will significantly reduce the current information void that must be filled to quantitate contaminant migration rates and model the exposure implications of such migration.

5.2. Insights from the Current Investigation

The specific scenario used for this preliminary investigation involved a controlled point release of a surrogate contaminant over a period of 1.25 hours. Although this scenario does not necessarily represent any specific product or contaminant, the experimental results have a number of implications for passive exposures and modeling thereof. Contaminant concentrations were generally 3 to 4 times higher in the room of release than in areas where passive exposures could occur, but concentrations in the other areas were distinguishably above background levels within 1 hour after the release was initiated. Further, spatial uniformity in concentrations throughout the main floor of the research house was approached within 45 to 60 minutes after the end of release period, during which time concentrations near the release area receded and concentrations in other areas continued to rise. Interestingly, a single-chamber model--similar to that currently used in OTS assessments of active exposures in residential environments--more closely approximated passive than active exposures; use of a multichamber model resulted in better estimation of each type of exposure.

Through detailed spatial and temporal monitoring, the research house experiments described and analyzed in this report have provided substantial insights into short-term contaminant migration patterns, but were restricted to one release scenario. Further experiments are needed to address the following types and conditions of simulated product use:

- Type of release--point versus area (e.g., wall or floor);
- Location of release;
- Duration of release;
- Status of interior doors (open or closed);
- Status of windows and exhaust fans; and
- Season and operation of heating/cooling systems.

Covering all possible combinations of these conditions would require a prohibitively large number of experiments; however, all combinations are not needed to obtain vital insights. The number of experiments could be substantially reduced, for example, by limiting the next round of investigation to (1) a standard type, duration, and location of release, but under different conditions relating to interior doors, windows, exhaust fans, and heating/cooling system operation, and (2) varying types, durations, or locations of release for a single set of conditions. Results from a recent EPA-sponsored consumer survey (Westat 1987) can be used to help determine the most common conditions surrounding product use.

To facilitate the conduct of experiments for a broader set of simulated product usage scenarios, a detailed stationary monitoring network needs to be established in the research houses; this can be accomplished by expanding the number of monitoring sites at the sacrifice of vertical detail at each site. An illustrative array of the CO detectors used in this investigation for such a network is given in Figure 27; monitoring sites in the bedrooms, living room, and downstairs living area represent probable receptor locations, whereas sites in the stairway and hallway areas represent likely pathways of contaminant migration.

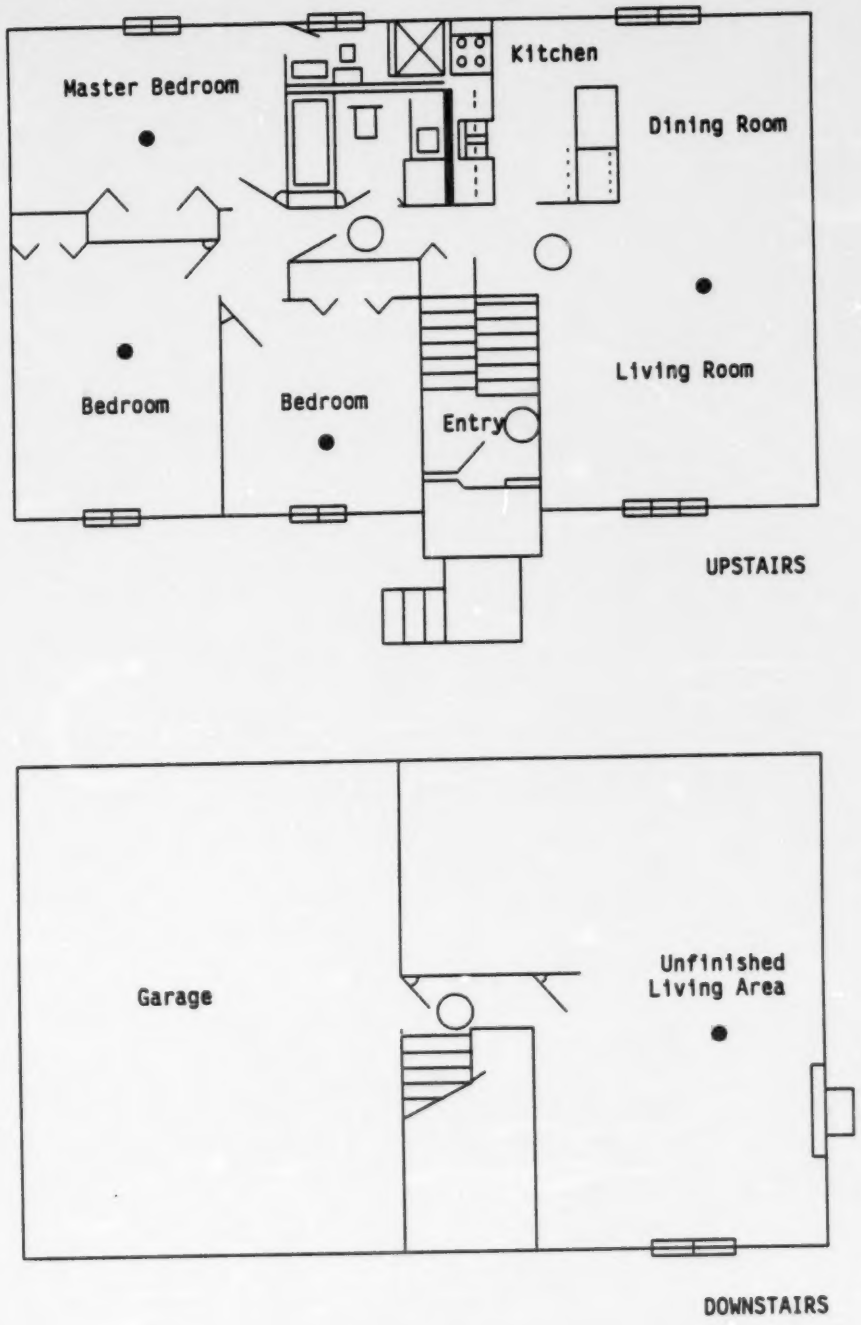


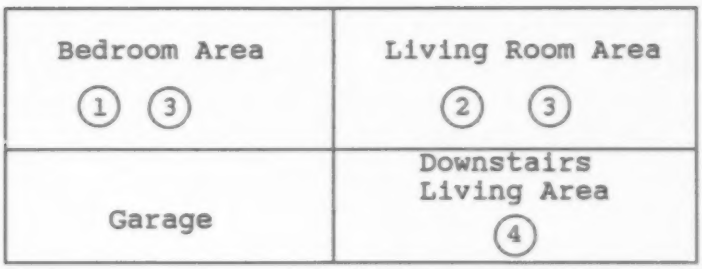
Figure 27. Illustrative monitoring array for future contaminant migration experiments (filled circles represent probable receptor locations; empty circles represent likely migration routes).

Providing a linkage between these experimental results and the PFT data base is vital to the ultimate goal of improving the accuracy and generalizability of consumer exposure models. Consequently, future experiments should include PFT measurements and real-time multiple tracer measurements as a standard component. An illustrative array of the four available types of PFT sources is given in Figure 28; this particular array will (1) enable quantitation of average airflows among the bedroom, living room, and downstairs areas and (2) provide a means of assessing whether flows between bedroom and living room areas can be inferred from upstairs-downstairs flows (important because, in many cases for multistory structures, PFT sources are configured to provide estimates of flows between but not within stories).

The transferability of results from research houses to a variety of housing types can be significantly aided by replicating selected research house experiments in the following types of structures:

- Single-story, slab-on-grade structure;
- Single-story structure with basement;
- Multistory above-grade structure (attached and detached); and
- Apartment unit.

Structures inhabited by colleagues or acquaintances could be used for pretests of this approach in a limited number of settings. As little as one structure of each type can provide substantial insights regarding not only the transferability of research house results but also the need for broader surveys of this type. Including a detailed temporal and spatial monitoring network in each house and making simultaneous PFT measurements will strengthen the linkage between the detailed research house results and the time-averaged PFT results that are available for a greater variety of structure types.



Note: Source types (3) and (4) represent a commonly used array of PFT sources for estimating flows between upstairs and downstairs areas; addition of source types (1) and (2) enables estimation of flows among three areas--bedrooms, living room, and downstairs--and can be used to assess whether flows between bedrooms and living room could be properly inferred if only source types (3) and (4) had been used.

Figure 28. Proposed array of PFT sources for future contaminant migration experiments.

6. CONCLUSIONS AND RECOMMENDATIONS

Major findings and conclusions stemming from the study results and modeling efforts given in Sections 3 and 4 are summarized in Section 6.1. Recommendations drawn from the discussion given in Section 5 are outlined in Section 6.2.

6.1. Conclusions

The major findings and conclusions from this preliminary investigation are as follows:

- During the 1.25-hour period when contaminant release from a consumer product in the master bedroom was simulated, resultant concentrations were 3 to 4 times higher in the area of the release than in other upstairs areas of the house.

- Within 45 to 60 minutes following the end of the contaminant-release period, concentrations throughout the upstairs of the house approached spatial uniformity, even though the central air circulation fan that would have promoted contaminant migration was kept off as part of the experimental design.

- Vertical gradients in contaminant concentrations were most pronounced and variable in the release area and along the migration path in the hallway, suggesting that a fairly complex and somewhat variable system of forces is involved in the mixing and transport of contaminants.

- Concentrations at potential passive exposure sites such as the living room and bedrooms adjacent to the release area were generally similar in magnitude, even during the release period; greater variations were observed during afternoon than morning experiments, possibly due to changing forces at play around sunset.

- Some evidence of contaminant migration downstairs was observed during selected experiments; however, even in these cases, downstairs concentrations were substantially lower than those upstairs.

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- Application of a one-zone model similar to that used for current OTS exposure assessments resulted in good estimates of passive exposure but substantial underestimation of active exposure.

- Application of a two-zone model resulted in good estimates of both active and passive exposures upstairs; thus, even though a complex set of forces may be involved in contaminant mixing and transport, the concept of treating general airflow patterns as a steady-state condition into which consumer-product emissions are injected and transported appears valid and useful for improving exposure estimates.

- The success of the two-zone modeling effort in estimating exposures for the release scenario examined under this investigation suggests that PFT measurement results coupled with continuing experiments in research houses will provide a means of substantially improving exposure estimates for a variety of scenarios relating to use of consumer products in residential environments.

6.2. Recommendations

A broader array of experiments should be conducted to investigate contaminant migration for different types of releases and surrounding conditions. Scenarios studied at the research house should be expanded in terms of (1) the type, location, and duration of release and (2) the status of interior doors, windows, exhaust fans, and heating/cooling system. A detailed stationary monitoring network should be established for these experiments and measurements of time-varying and time-averaged interzonal airflows should be included as a routine component of the monitoring design. Such experiments will improve our understanding of contaminant migration patterns and exposure implications for the greater variety of release types and surrounding conditions that prevail in residential settings.

The method of point release used for the current investigation should be repeated with the new monitoring design. A point-source release of 1.25-hour duration should be repeated in the master bedroom, first with the central air circulation fan off at all times and then with the fan on at all times. These two conditions should then be repeated with the release point moved to the living room and then downstairs. Next, a different

type of release (e.g., from an area source such as a wall or floor) should be performed under similar conditions to evaluate commonalities in migration patterns across different release types. Following this sequence of experiments, the release type and location should remain fixed but other conditions (e.g., interior doors, windows, and exhaust fans) should be varied, first one at a time and then in selected combinations. Finally, selected types of experiments should be conducted with a consumer product in use--one for which detailed monitoring of the associated contaminant(s) can be performed at a reasonable cost.

Selected types of research house experiments should be replicated in a limited number of other structures to aid in transferring the research results to various residential settings. The number of scenarios should be restricted to four at most, such as two release locations for each of two surrounding conditions. Other types of structures should include single-story detached residences with and without a basement, a multistory above-grade residence, and an apartment unit. The detailed monitoring network used at the research house should be temporarily relocated to these other residences for this phase of research.

As soon the the BNL data base of PFT measurement results has been unified in a computer-accessible format, analytical efforts should be initiated. The range and distribution of air infiltration rates in different types of structures in different geographic areas and at different times of the year should be determined from the data base. Based on this analysis, characteristic airflows should be estimated for specific structure-area-season combinations as inputs to future modeling efforts. The analysis should also assess whether any systematic relationship exists between the magnitudes of air infiltration rates and internal airflows.

In parallel with the research efforts described above, activities to refine and improve currently used exposure assessment models should be initiated. This process should begin with the development of a generalized multichamber model and continue with refinements and expansions, as critical inputs are obtained from the research efforts recommended above.

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Appendix A

INDOOR AIR QUALITY MODELING CONCEPTS AND FORMULATIONS*

* The contents of this appendix have been excerpted from "Scoping and Feasibility Study: Room-to-Room Contaminant Migration and OTS Indoor Air Exposure Assessments," GEOMET Report No. IE-1820, submitted to the Office of Toxic Substances, September 1987.

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The most widely used models for calculating contaminant concentrations indoors represent the airspace of interest as a single well-stirred chamber or as a series of interconnected chambers. Rather than map the three-dimensional velocity and dispersion field, these models track the amount of the contaminant in the chamber(s) in terms of the mass balance defined by generation; by inflow and outflow; and, for reactive contaminants, by removal to sinks.

Because the mass balance approach incorporates important physical factors and processes directly, it has become the main theoretical framework for indoor air quality simulations. The general mathematical expression of the mass balance is in the form of a differential equation that, in solved form, constitutes a user-implemented model. Such implementations include code-intensive computer programs featuring numerical techniques (Nazzaroff and Cass 1986) as well as simplified approaches involving analytical solutions applied through programs on desk-top computers (Nagda et al. 1985).

Single-chamber models define a given air space (e.g., a room, a group of rooms or zone, or an entire building) as a single well-mixed volume. To extend the single-chamber approach to multiple chambers for quantifying zone-to-zone migration, the indoor volume must be represented as a network of interconnected chambers. Contaminant mass balance is carried out for each of these chambers; communicating flows with other chambers (Figure A-1) are also considered.

Because conditions in a given chamber are determined by interactions with all other connecting chambers, the multichamber model is stated as a system of simultaneous equations. The mathematical framework for the multichamber description has been reviewed by Sinden (1978) and by Sandberg (1984). General equational forms for the single- and multichamber models are presented in Table A-1.

From an operational standpoint, the most difficult decisions concern appropriate model scenarios in terms of chambers and airflows. The general patterns are of three basic types: (1) air exchange between chambers and outdoors (Qio, Qoi), (2) chamber-to-chamber airflows (Qij), and (3) air circulation within chambers. These patterns are illustrated in Figure A-2. The definition of a chamber can entail (1) the entire building, (2) a zone or group of rooms, (3) a single room, or (4) a part of a room.

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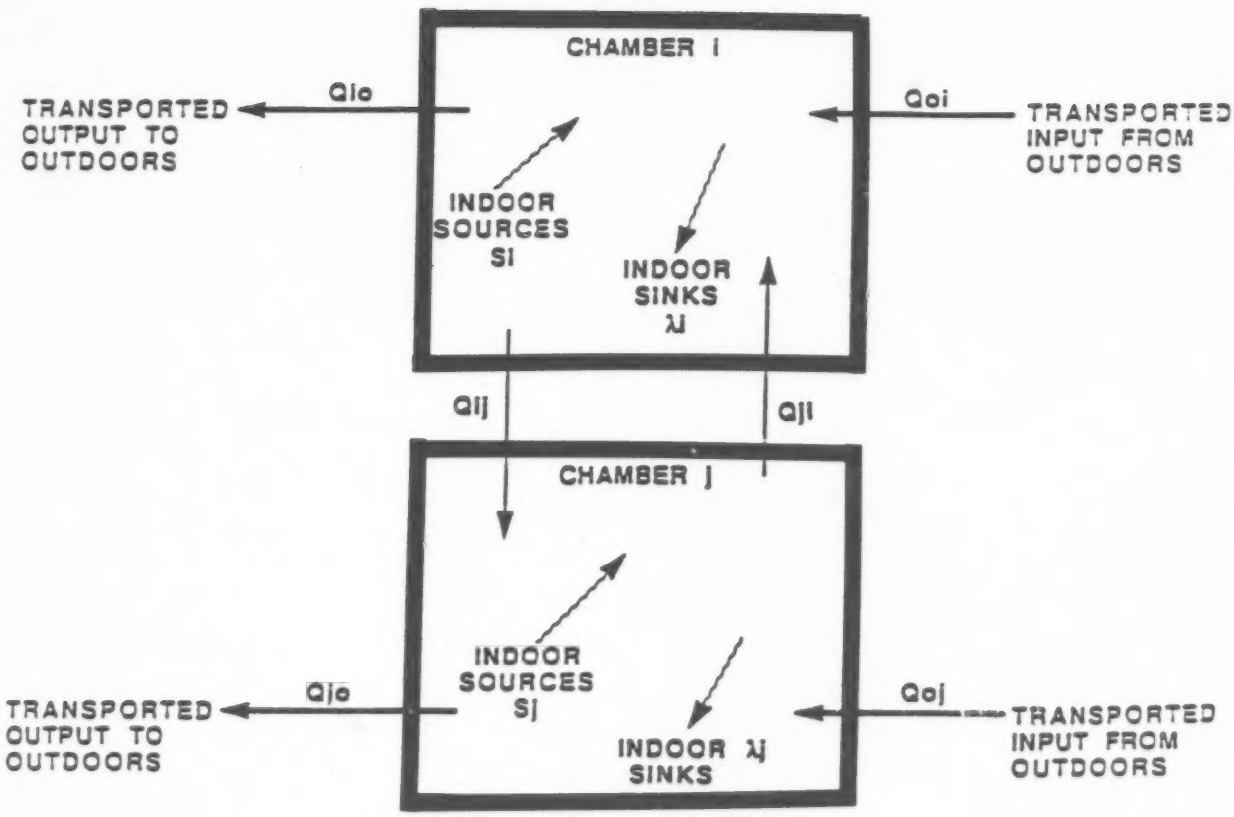
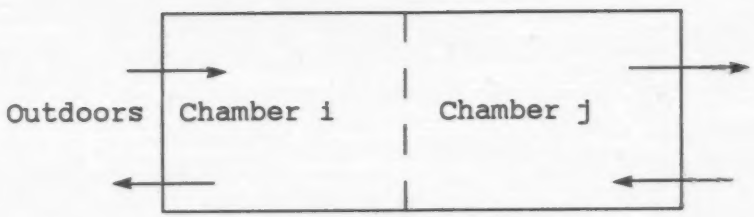


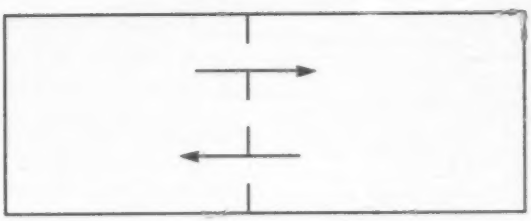
Figure A-1. Basic mass balance relationships for multichamber approach.

Table A-1. Single-Chamber and Multichamber Model Summary

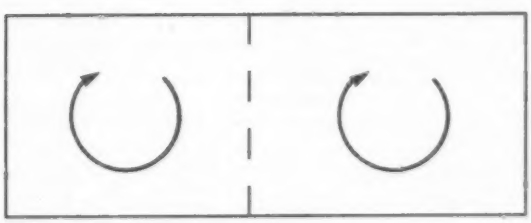
Single-chamber	Multichamber
$V \frac{dC_{in}}{dt} = G + Q_{oi}C_{out} - Q_{io}C_{in}$	$V_i \frac{dC_i}{dt} = G_i + \sum_{j \neq i}^{n} Q_{ji}C_j - \sum_{j \neq i}^{n} Q_{ij}C_i$
INPUTS	INPUTS
G = Source release rate (g/h) V = Volume (m^3) Q_{oi} = Flow from outdoors (m^3/h) Q_{io} = Flow to outdoors (m^3/h) C_{out} = Outdoor concentration (g/m^3)	G_i = Source release rate in ith chamber (g/h) V_i = Volume of ith chamber (m^3) Q_{ji} = Flow from jth to ith chamber (m^3/h) Q_{ij} = Flow from ith to jth chamber (m^3/h) C_j - Concentration in jth chamber (g/m^3)
AIR MASS BALANCE	AIR MASS BALANCE
$Q_{io} = Q_{oi}$	$\sum_{j \neq i}^{n} Q_{ji} = \sum_{j \neq i}^{n} Q_{ij}$
OUTPUT	OUTPUT
C_{in} - Indoor concentration (g/m^3)	C_i - Concentration in ith chamber (g/m^3)



1. Air Exchange
   - Natural Infiltration
   - Natural Ventilation
   - Mechanical Ventilation
   - Local Exhaust



2. Chamber-to-chamber Airflow
   - Convective Circulation
   - Advective Circulation
   - Mechanical Circulation



3. Local Circulation
   - Convective Mixing
   - Mechanical Mixing

Figure A-2. Basic patterns of air motion to be considered in modeling.

Local circulation relates to the completeness of mixing. In the single-chamber description, effective volume and mixing factors are sometimes employed to refine concentration estimates (Nagda et al. 1987). Within the multichamber description, incomplete mixing signals a need for designation of additional chambers. For residential structures, this primarily involves defining zones versus individual rooms. Relatively little quantitative work has been reported that would lead to general rules for subdividing individual rooms to accommodate vertical stratification.

Expanding the model perspective to the multichamber description allows the exposure analyst to consider active exposure and passive exposure simultaneously at the relatively minor cost of additional complexity in calculations. The primary needs for implementation center on defining attributes of the exposure scenarios that relate to volumes and flows.

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